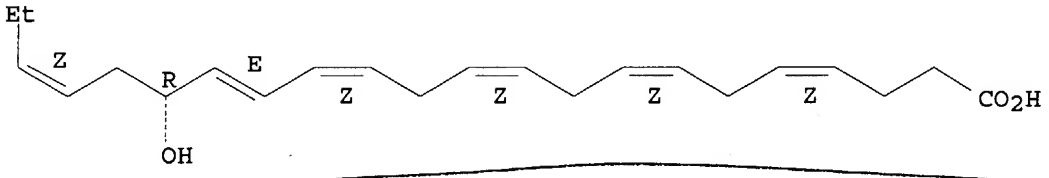
=> d ibib abs hitstr l28 1-57

L28 ANSWER 1 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:977402 HCAPLUS
TITLE: Novel Docosanoids Inhibit Brain Ischemia-Reperfusion-mediated Leukocyte Infiltration and Pro-inflammatory Gene Expression. [Erratum to document cited in CA139:379337]
AUTHOR(S): Marcheselli, Victor L.; Hong, Song; Lukiw, Walter J.; Tian, Xiao Hua; Gronert, Karsten; Musto, Alberto; Hardy, Mattie; Gimenez, Juan M.; Chiang, Nan; Serhan, Charles N.; Bazan, Nicolas G.
CORPORATE SOURCE: Neurosci. Cent. Excellence, Dep. Ophthalmol., Louisiana State Univ. Health Sci. Cent., New Orleans, LA, 70112, USA
SOURCE: Journal of Biological Chemistry (2003), 278(51), 51974
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal; Errata
LANGUAGE: English
AB An erratum.
IT INDEXING IN PROGRESS
IT **155976-53-7**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(novel docosanoids inhibit brain ischemia-reperfusion-mediated leukocyte infiltration and pro-inflammatory gene expression (Erratum))
RN 155976-53-7 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, (4Z,7Z,10Z,13Z,15E,17R,19Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L28 ANSWER 2 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:850857 HCAPLUS
DOCUMENT NUMBER: 139:379337
TITLE: Novel Docosanoids Inhibit Brain Ischemia-Reperfusion-mediated Leukocyte Infiltration and Pro-inflammatory Gene Expression
AUTHOR(S): Marcheselli, Victor L.; Hong, Song; Lukiw, Walter J.; Tian, Xiao Hua; Gronert, Karsten; Musto, Alberto; Hardy, Mattie; Gimenez, Juan M.; Chiang, Nan; Serhan, Charles N.; Bazan, Nicolas G.
CORPORATE SOURCE: Neurosci. Cent. Excellence, Dep. Ophthalmol., Louisiana State Univ. Health Sci. Cent., New Orleans, LA, 70112, USA
SOURCE: Journal of Biological Chemistry (2003), 278(44), 43807-43817
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular

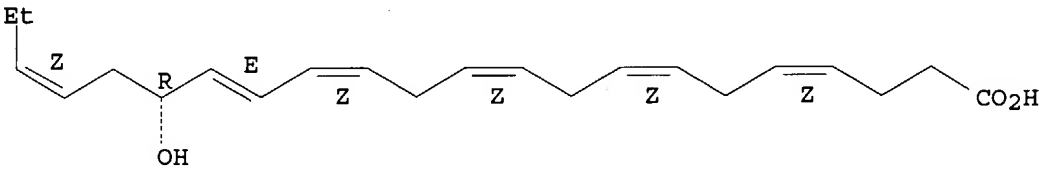
Biology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Ischemic stroke triggers lipid peroxidn. and neuronal injury. Docosahexaenoic acid released from membrane phospholipids during brain ischemia is a major source of lipid peroxides. Leukocyte infiltration and pro-inflammatory gene expression also contribute to stroke damage. In this study using lipidomic anal., we have identified stereospecific messengers from docosahexaenoate-oxygenation pathways in a mouse stroke model. Aspirin, widely used to prevent cerebrovascular disease, activates an addnl. pathway, which includes the 17R-resolvins. The newly discovered brain messenger 10,17S-docosatriene potently inhibited leukocyte infiltration, NFκB, and cyclooxygenase-2 induction in exptl. stroke and elicited neuroprotection. In addition, in neural cells in culture, this lipid messenger also inhibited both interleukin 1β-induced NFκB activation and cyclooxygenase-2 expression. Thus, the specific novel bioactive docosanoids generated in vivo counteract leukocyte-mediated injury as well as pro-inflammatory gene induction. These results challenge the view that docosahexaenoate only participates in brain damage and demonstrate that this fatty acid is also the endogenous precursor to a neuroprotective signaling response to ischemia-reperfusion.

IT **155976-53-7**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(novel docosanoids inhibit brain ischemia-reperfusion-mediated leukocyte infiltration and pro-inflammatory gene expression)

RN 155976-53-7 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, (4Z,7Z,10Z,13Z,15E,17R,19Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 3 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:511135 HCAPLUS
DOCUMENT NUMBER: 139:79114
TITLE: Eicosapentaenoic acid and docosahexaenoic acid analogs induction of host defense against bacteria
INVENTOR(S): Serhan, Charles N.; Colgan, Sean P.
PATENT ASSIGNEE(S): The Brigham and Women's Hospital, USA
SOURCE: PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003053423	A2	20030703	WO 2002-US40586	20021218

NPA

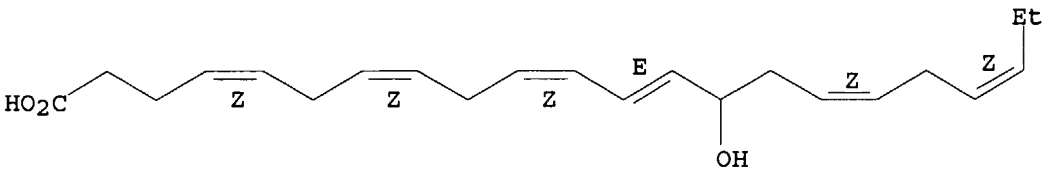
WO 2003053423 A3 20040226
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
US 2003191184 A1 20031009 US 2002-323867 20021218
US 2003195248 A1 20031016 US 2002-323591 20021218
PRIORITY APPLN. INFO.: US 2001-342138P P 20011218
OTHER SOURCE(S): MARPAT 139:79114

AB Methods to cause tissue, such as mucosal cells, to express increased amts. of bactericidal permeability increasing protein (BPI) are described. Various BPI inducing agents include eicosapentaenoic acid (EPA) analogs and docosahexaenoic acid (DHA) analogs. Thus, 18R-EPA analogs induced the formation of BPI. Results demonstrated quant. PCR for BPI in epithelial cells.

IT **87042-40-8 90780-51-1 90780-52-2**
90780-53-3 90906-41-5 356041-27-5
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(eicosapentaenoic acid and docosahexaenoic acid analogs induction of host defense against bacteria)

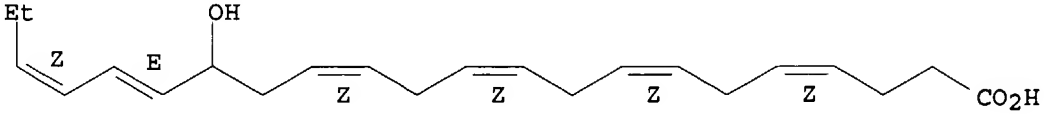
RN 87042-40-8 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



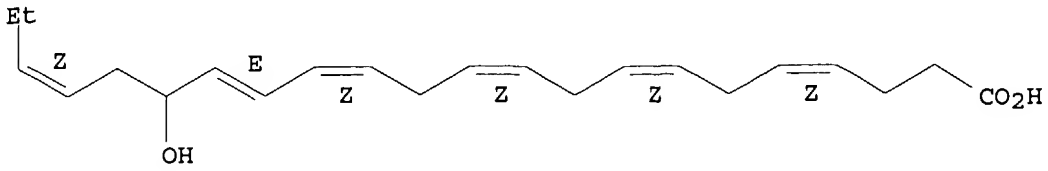
RN 90780-51-1 HCAPLUS
CN 4,7,10,13,17,19-Docosahexaenoic acid, 16-hydroxy-, (4Z,7Z,10Z,13Z,17E,19Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



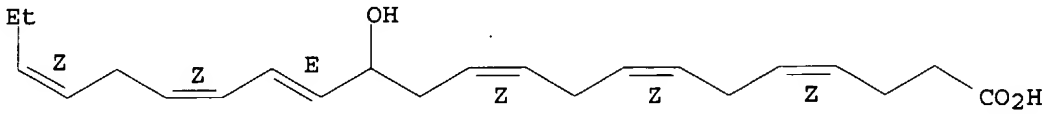
RN 90780-52-2 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, (4Z,7Z,10Z,13Z,15E,19Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 90780-53-3 HCAPLUS
CN 4,7,10,14,16,19-Docosahexaenoic acid, 13-hydroxy-, (4Z,7Z,10Z,14E,16Z,19Z)-
(9CI) (CA INDEX NAME)

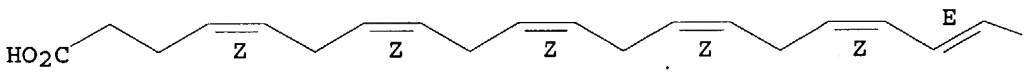
Double bond geometry as shown.



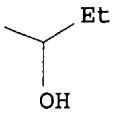
RN 90906-41-5 HCAPLUS
CN 4,7,10,13,16,18-Docosahexaenoic acid, 20-hydroxy-, (4Z,7Z,10Z,13Z,16Z,18E)-
(9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



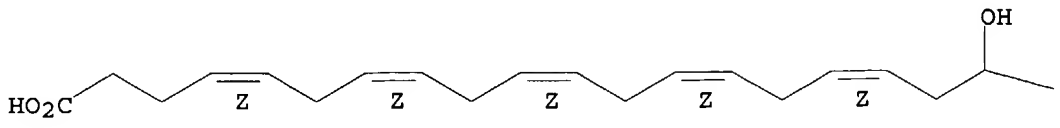
PAGE 1-B

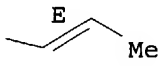


RN 356041-27-5 HCAPLUS
CN 4,7,10,13,16,20-Docosahexaenoic acid, 19-hydroxy-, (4Z,7Z,10Z,13Z,16Z,20E)-
(9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A





L28 ANSWER 4 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:304562 HCAPLUS
DOCUMENT NUMBER: 139:177077
TITLE: Novel Docosatrienes and 17S-Resolvins Generated from Docosahexaenoic Acid in Murine Brain, Human Blood, and Glial Cells
AUTHOR(S): Hong, Song; Gronert, Karsten; Devchand, Pallavi R.; Moussignac, Rose-Laure; Serhan, Charles N.
CORPORATE SOURCE: Perioperative and Pain Medicine, Department of Anesthesiology, Center for Experimental Therapeutics and Reperfusion Injury, Brigham and Women's Hospital and Harvard Medical School, Boston, MA, 02115, USA
SOURCE: Journal of Biological Chemistry (2003), 278(17), 14677-14687
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English

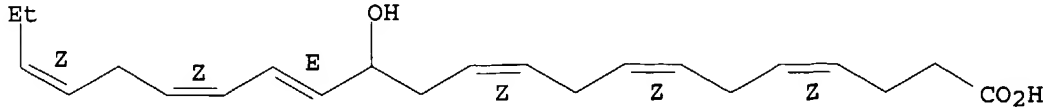
NRA

AB Docosahexaenoic acid (DHA, C22:6) is highly enriched in brain, synapses, and retina and is a major ω-3 fatty acid. Deficiencies in this essential fatty acid are reportedly associated with neuronal function, cancer, and inflammation. Here, using new lipid analyses employing high performance liquid chromatog. coupled with a photodiode-array detector and a tandem mass spectrometer, a novel series of endogenous mediators was identified in blood, leukocytes, brain, and glial cells as 17S-hydroxy-containing docosanoids denoted as docosatrienes (the main bioactive member of the series was 10,17S-docosatriene) and 17S series resolvins. These novel mediators were biosynthesized via epoxide-containing intermediates and proved potent (pico- to nanomolar range) regulators of both leukocytes reducing infiltration in vivo and glial cells blocking their cytokine production These results indicate that DHA is the precursor to potent protective mediators generated via enzymic oxygenations to novel docosatrienes and 17S series resolvins that each regulate events of interest in inflammation and resolution

IT **90780-53-3 92693-03-3**
RL: ANT (Analyte); BSU (Biological study, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study)
(docosatrienes and 17S-resolvins generated from docosahexaenoic acid in murine brain, human blood, and glial cells)

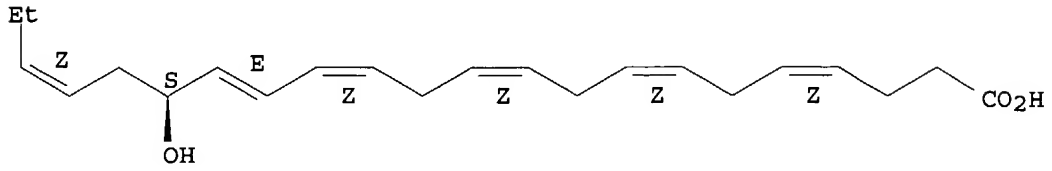
RN 90780-53-3 HCAPLUS
CN 4,7,10,14,16,19-Docosahexaenoic acid, 13-hydroxy-, (4Z,7Z,10Z,14E,16Z,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



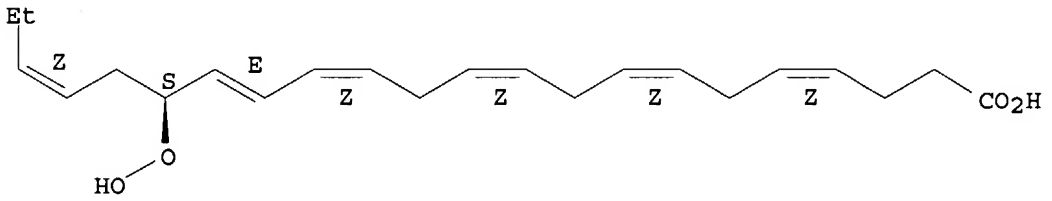
RN 92693-03-3 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, [S-(E,Z,Z,Z,Z,Z)]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



IT **123673-33-6**
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); BIOL (Biological study)
(docosatrienes and 17S-resolvins generated from docosahexaenoic acid in murine brain, human blood, and glial cells)
RN 123673-33-6 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroperoxy-, (4Z,7Z,10Z,13Z,15E,17S,19Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 5 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:977645 HCAPLUS
DOCUMENT NUMBER: 138:33381
TITLE: PPARγ agonistic medicinal compositions
INVENTOR(S): Tamai, Tadakazu; Yoshikai, Kazuyoshi; Nishikawa, Masazumi
PATENT ASSIGNEE(S): Maruha Corporation, Japan
SOURCE: PCT Int. Appl., 26 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002102364	A1	20021227	WO 2002-JP6066	20020618

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,

NPN

LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1407767 A1 20040414 EP 2002-733509 20020618
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

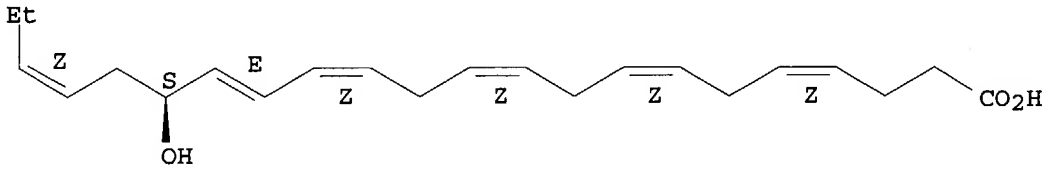
PRIORITY APPLN. INFO.: JP 2001-182731 A 20010618
WO 2002-JP6066 W 20020618

AB PPARγ agonistic medicinal compns. containing a hydroxylated derivative of a highly unsatd. fatty acid having a C20-22 carbon chain or a pharmaceutically acceptable salt thereof, preferably PPARγ agonistic medicinal compns. containing a hydroxylated derivative of docosahexaenoic acid (DHA) or eicosapentaenoic acid (EPA) or a pharmaceutically acceptable salt thereof; and use of these PPAR: γ agonistic compns. in treating circulatory diseases, arteriosclerosis, lipid metabolic diseases, diabetes and inflammatory diseases.

IT **92693-03-3P 119433-37-3P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(PPARγ agonistic unsatd. fatty acids for treatment of circulatory diseases, arteriosclerosis, lipid metabolic diseases, diabetes and inflammatory diseases)

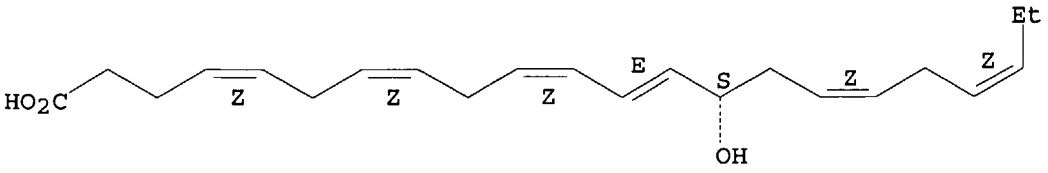
RN 92693-03-3 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, [S-(E,Z,Z,Z,Z,Z)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 119433-37-3 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,14S,16Z,19Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

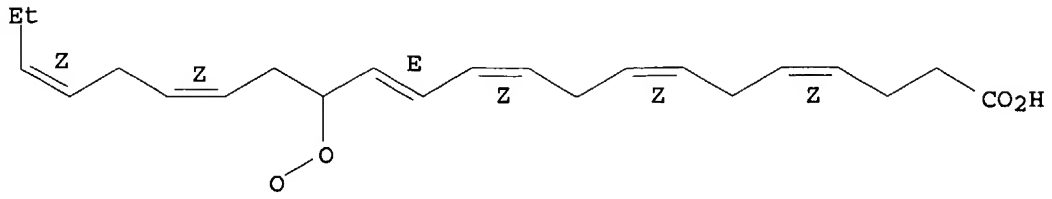
L28 ANSWER 6 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:744023 HCAPLUS
DOCUMENT NUMBER: 138:23073
TITLE: Formation of Highly Reactive A-ring and J-ring Isoprostane-like Compounds (A4/J4-neuroprostanes) in Vivo from Docosahexaenoic Acid
AUTHOR(S): Fam, Samuel S.; Murphey, Laine J.; Terry, Erin S.; Zackert, William E.; Chen, Yan; Gao, Ling; Pandalai, Saurabh; Milne, Ginger L.; Roberts, L. Jackson; Porter, Ned A.; Montine, Thomas J.; Morrow, Jason D.
CORPORATE SOURCE: Departments of Medicine, Pharmacology, Chemistry, and Pathology, Vanderbilt University School of Medicine, Nashville, TN, 37232, USA
SOURCE: Journal of Biological Chemistry (2002), 277(39), 36076-36084
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Free radical-initiated oxidant injury and lipid peroxidn. have been implicated in a number of neural disorders. Docosahexaenoic acid is the most abundant unsatd. fatty acid in the central nervous system. The authors have shown previously that this 22-carbon fatty acid can yield, upon oxidation, isoprostane-like compds. termed neuroprostanes, with E/D-type prostane rings (E4/D4-neuroprostanes). Eicosanoids with E/D-type prostane rings are unstable and dehydrate to cyclopentenone-containing compds. possessing A-type and J-type prostane rings, resp. The authors thus explored whether cyclopentenone neuroprostanes (A4/J4-neuroprostanes) are formed from the dehydration of E4/D4-neuroprostanes. Indeed, oxidation of docosahexaenoic acid in vitro increased levels of putative A4/J4-neuroprostanes 64-fold from 88 to 5463 ng/mg docosahexaenoic acid. Chemical approaches and liquid chromatog./electrospray ionization tandem mass spectrometry definitively identified them as A4/J4-neuroprostanes. The authors subsequently showed these compds. are formed in significant amts. from a biol. source, rat brain synaptosomes. A4/J4-neuroprostanes increased 13-fold, from a basal level of 89 ng/mg protein to 1187 ng/mg, upon oxidation The authors also detected these compds. in very large amts. in fresh brain tissue from rats at levels of 97 ng/g brain tissue and from humans at levels of 98 ng/g brain tissue, quantities that are nearly an order of magnitude higher than other classes of neuroprostanes. Because of the fact that A4/J4-neuroprostanes contain highly reactive cyclopentenone ring structures, it would be predicted that they readily undergo Michael addition with glutathione and adduct covalently to proteins. Indeed, incubation of A4/J4-neuroprostanes in vitro with excess glutathione resulted in the formation of large amts. of adducts. Thus, these studies have identified novel, highly reactive A/J-ring isoprostane-like compds. that are derived from docosahexaenoic acid in vivo.

IT **478298-64-5 478298-68-9 478298-70-3 478298-71-4**
RL: ADV (Adverse effect, including toxicity); BSU (Biological study, unclassified); BIOL (Biological study)
(intermediate; formation of highly reactive A-ring and J-ring isoprostane-like compds. (A4/J4-neuroprostanes) in vivo from docosahexaenoic acid in relation to free radical-initiated oxidant injury/lipid peroxidn. in neural disorders)

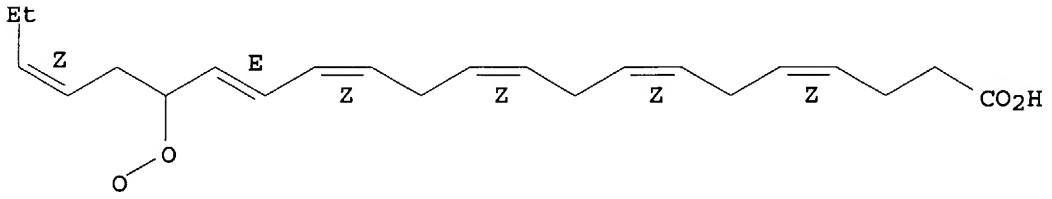
RN 478298-64-5 HCAPLUS
CN 2,4,7,10-Tridecatetraenyldioxy, 13-carboxy-1-(2Z,5Z)-2,5-octadienyl-, (2E,4Z,7Z,10Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



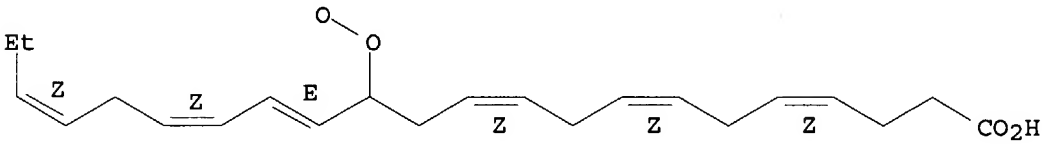
RN 478298-68-9 HCAPLUS
CN 2,4,7,10,13-Hexadecapentaenyldioxy, 16-carboxy-1-(2Z)-2-pentenyl-, (2E,4Z,7Z,10Z,13Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



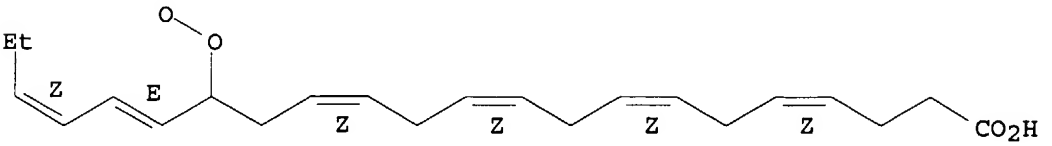
RN 478298-70-3 HCAPLUS
CN 3,6,9-Dodecatrienyldioxy, 12-carboxy-1-(1E,3Z,6Z)-1,3,6-nonatrienyl-, (3Z,6Z,9Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 478298-71-4 HCAPLUS
CN 3,6,9,12-Pentadecatetraenyldioxy, 15-carboxy-1-(1E,3Z)-1,3-hexadienyl-, (3Z,6Z,9Z,12Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 7 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:849682 HCAPLUS
DOCUMENT NUMBER: 136:147175
TITLE: Monohydroxylated fatty acid content in peripheral

blood mononuclear cells and immune status of people at long times after the Chernobyl accident

AUTHOR(S): Chumak, Anatoliy; Thevenon, Chantal; Gulaya, Nadya; Guichardant, Michel; Margitich, Victor; Bazyka, Dimitry; Kovalenko, Alexander; Lagarde, Michel; Prigent, Annie-France

CORPORATE SOURCE: INSERM, Biochimie et Pharmacologie INSA Lyon, Villeurbanne, 69621, Fr.

SOURCE: Radiation Research (2001), 156(5, Pt. 1), 476-487
CODEN: RAREAE; ISSN: 0033-7587

PUBLISHER: Radiation Research Society

DOCUMENT TYPE: Journal

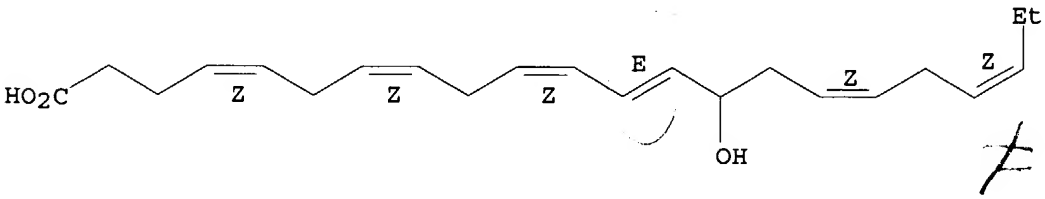
LANGUAGE: English

AB The monohydroxylated fatty acid content of peripheral blood mononuclear cells from 23 cleanup workers and 16 unexposed individuals was studied in relation to their immune status after the Chernobyl accident. Men with absorbed doses below 0.32 Gy showed higher levels of free and esterified 12-hydroxyeicosatetraenoic acid (12-HETE) than unexposed men, whereas 15-HETE and the 17-hydroxy derivative of C22 fatty acid (17-OH 22), either free or esterified in phospholipids, were increased in a dose-dependent manner. The percentage of CD4-pos. cells was also increased significantly in heavily irradiated men, whereas the percentage of CD8-pos. cells tended to decrease with dose. Furthermore, the absolute count of CD4-pos. cells was correlated pos. with the amount of esterified 15-HETE in the phospholipid fraction of the mononuclear cells and with the total 15-HETE. These results show for the first time that the accumulation of autoxidized/lipoxygenase products of polyunsatd. fatty acids in the mononuclear cells of irradiated individuals was associated with immune imbalance. This may be the basis for certain late effects of radiation such as autoimmune disorders, somatic and neoplastic diseases, and early aging.

IT **87042-40-8 90780-52-2**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(monohydroxylated fatty acid content in peripheral blood mononuclear cells and immune status of people after Chernobyl accident)

RN 87042-40-8 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)-(9CI) (CA INDEX NAME)

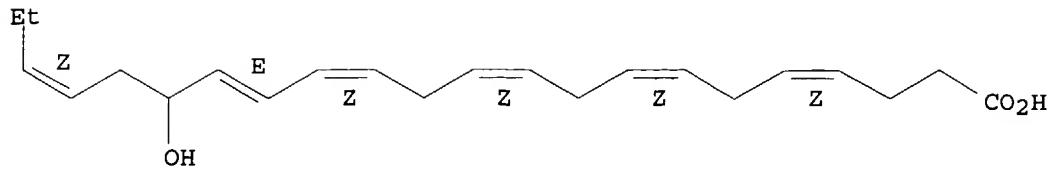
Double bond geometry as shown.



isomer

RN 90780-52-2 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, (4Z,7Z,10Z,13Z,15E,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



102(b)
Claim 29

REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 8 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:617963 HCAPLUS
DOCUMENT NUMBER: 135:190408
TITLE: Aspirin-triggered lipid mediators
INVENTOR(S): Serhan, Charles N.; Clish, Clary B.
PATENT ASSIGNEE(S): The Brigham and Women's Hospital, Inc., USA
SOURCE: PCT Int. Appl., 74 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001060778	A2	20010823	WO 2001-US5196	20010216
WO 2001060778	C2	20021024		
WO 2001060778	A3	20030116		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002055538	A1	20020509	US 2001-785866	20010216
US 6670396	B2	20031230		
EP 1296923	A2	20030402	EP 2001-910912	20010216
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003525880	T2	20030902	JP 2001-559832	20010216
US 2004059144	A1	20040325	US 2003-663061	20030912

PRIORITY APPLN. INFO.:
US 2000-183078P P 20000216
US 2000-238814P P 20001006
US 2001-785866 A3 20010216
WO 2001-US5196 W 20010216

OTHER SOURCE(S): MARPAT 135:190408

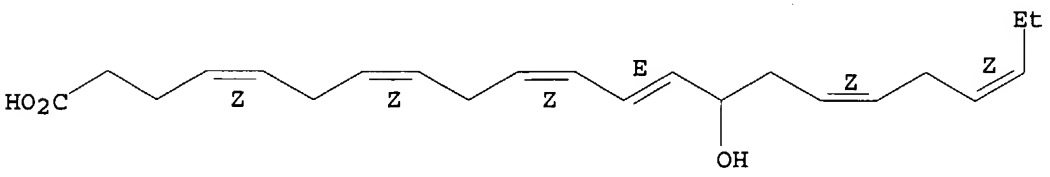
AB Aspirin triggered lipid mediators are disclosed which are useful for the treatment or prevention of inflammation associated with various diseases, including ischemia. The present invention provides that inflammatory exudates from mice treated with ω-3 PUFA and aspirin generate a novel array of bioactive lipid signals. Human endothelial cells with upregulated COX-2 treated with aspirin converted C20:5 w-3 to 18R-HEPE and 15R-HEPE. Each was used by polymorphonuclear leukocytes to generate sep. classes of novel trihydroxy-containing mediators, including 15R-lipoxin and 5,12,18R-triHEPE. These compds. were potent inhibitors of human

polymorphonuclear leukocyte transendothelial migration and infiltration in vivo.

IT **87042-40-8 90780-51-1 90780-52-2 90780-53-3 90906-41-5 356041-27-5**
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative) (lipid mediators generated by combination of ω-3 PUFA and aspirin)

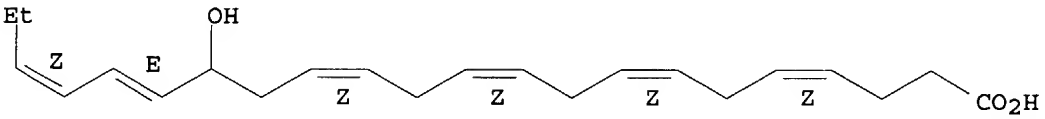
RN 87042-40-8 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



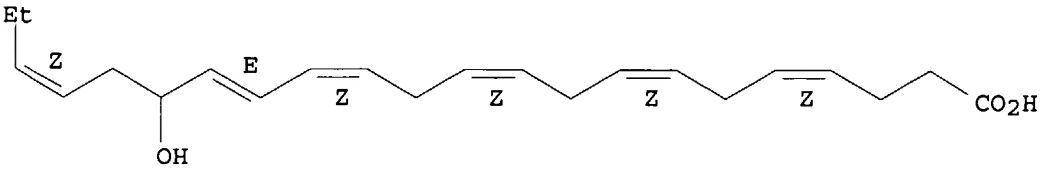
RN 90780-51-1 HCAPLUS
CN 4,7,10,13,17,19-Docosahexaenoic acid, 16-hydroxy-, (4Z,7Z,10Z,13Z,17E,19Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



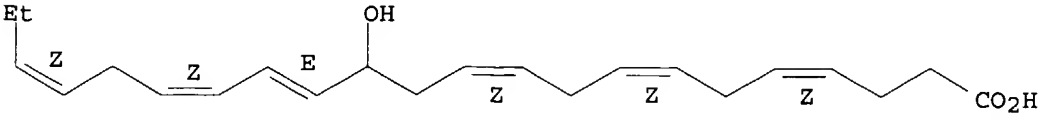
RN 90780-52-2 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, (4Z,7Z,10Z,13Z,15E,19Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 90780-53-3 HCAPLUS
CN 4,7,10,14,16,19-Docosahexaenoic acid, 13-hydroxy-, (4Z,7Z,10Z,14E,16Z,19Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

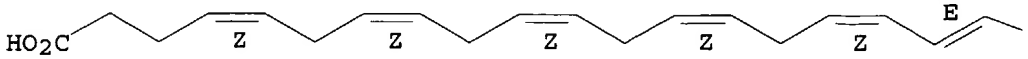


RN 90906-41-5 HCAPLUS

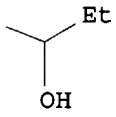
CN 4,7,10,13,16,18-Docosahexaenoic acid, 20-hydroxy-, (4Z,7Z,10Z,13Z,16Z,18E)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



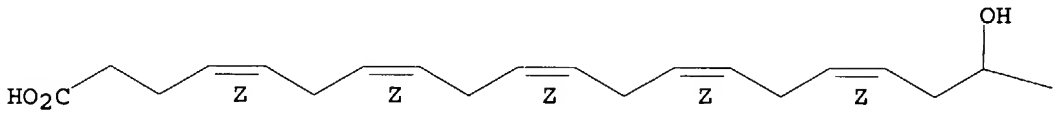
PAGE 1-B



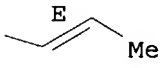
RN 356041-27-5 HCAPLUS
CN 4,7,10,13,16,20-Docosahexaenoic acid, 19-hydroxy-, (4Z,7Z,10Z,13Z,16Z,20E)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

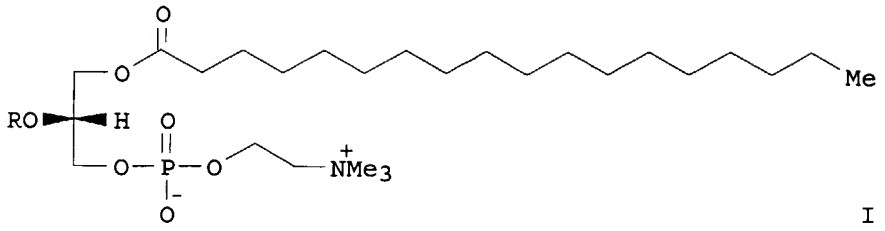


PAGE 1-B

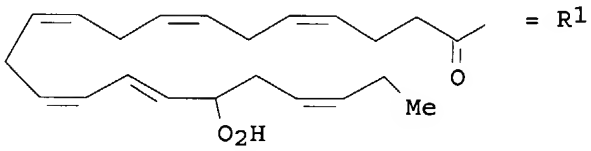


L28 ANSWER 9 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:374320 HCAPLUS
DOCUMENT NUMBER: 135:137640
TITLE: Synthesis and stability of phosphatidylcholines bearing polyenoic acid hydroperoxides at the sn-2 position
AUTHOR(S): Onyango, Arnold N.; Inoue, Takafumi; Nakajima, Shuhei; Baba, Naomichi; Kaneko, Takao; Matsuo, Mitsuyoshi; Shimizu, Sakayu
CORPORATE SOURCE: Department of Bioresources Chemistry Faculty of Agriculture, Okayama University, Okayama, 700-8530, Japan
SOURCE: Angewandte Chemie, International Edition (2001), 40(9), 1755-1757
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal

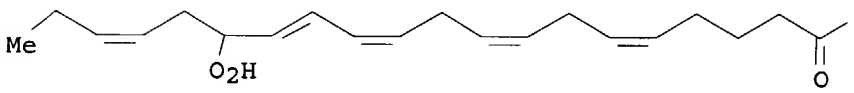
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:137640
GI



I



= R1



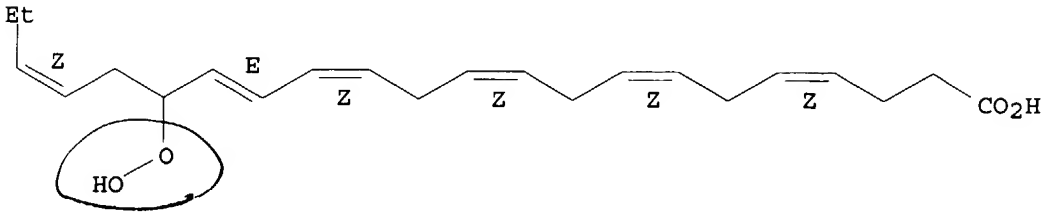
= R2

AB Two new phospholipid hydroperoxides I (R = R1, R2) were synthesized from docosahexaenoic acid (DHA) and eicosapentaenoic acid (EPA). The stability of the former is sufficient for storage and for use in biol. studies.

IT **70596-95-1P 351525-53-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and stability of phosphatidylcholines bearing polyenoic acid hydroperoxides at the sn-2 position)

RN 70596-95-1 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroperoxy-, (4Z,7Z,10Z,13Z,15E,19Z)- (9CI) (CA INDEX NAME)

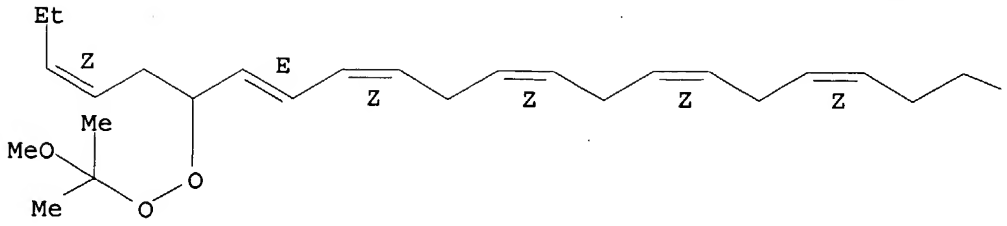
Double bond geometry as shown.



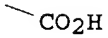
RN 351525-53-6 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-[(1-methoxy-1-methylethyl)dioxy]-, (4Z,7Z,10Z,13Z,15E,19Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 10 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:201254 HCAPLUS
DOCUMENT NUMBER: 131:16609
TITLE: The eicosanoid generating capacity of isolated cell populations from the gills of the rainbow trout, Oncorhynchus mykiss
AUTHOR(S): Holland, Jason W.; Taylor, Graham W.; Rowley, Andrew F.
CORPORATE SOURCE: School of Biological Sciences, University of Wales Swansea, Swansea, SA2 8PP, UK
SOURCE: Comparative Biochemistry and Physiology, Part C: Pharmacology, Toxicology & Endocrinology (1999), 122C(3), 297-306
CODEN: CBPCEE; ISSN: 0742-8413
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Rainbow trout gill filaments generated a wide range of eicosanoid products following calcium ionophore challenge. The putative lipoxygenase products were separated by reverse phase HPLC (RP-HPLC), while prostanoids were quantified by enzyme immunoassay. Three main monohydroxy compds. containing conjugated dienes were observed after RP-HPLC namely 12-(S) hydroxyeicosatetraenoic acid (12-HETE), 12-(S) hydroxyeicosapentaenoic acid (12-HEPE) and 14-(S) hydroxydocosahexaenoic acid (14-HDHE), derived from endogenous arachidonic, eicosapentaenoic and docosahexaenoic acids, resp. Their identification was confirmed by mass spectrometry. A further five compds. containing conjugated trienes were also observed but in lesser amts.

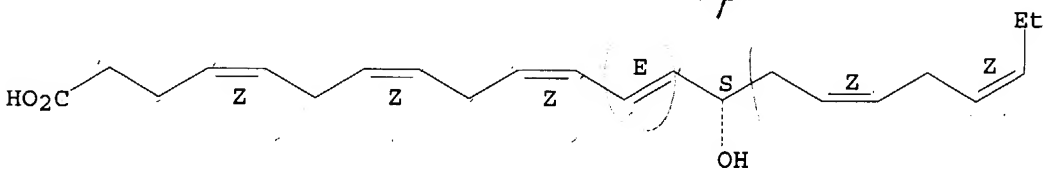
One of these products was identified as 8,15-dihydroxyeicosatetraenoic acid (8,15-DiHETE) based on its UV spectrum, co-elution with authentic standard on RP-HPLC and mass spectrometry. Overall, the generation of these products suggests the presence of 12- and possibly 15-lipoxygenase activities in trout gill acting on endogenous sources of fatty acid. To determine if the various cell types in trout gill had differing eicosanoid generating potential, gills were disrupted and the resultant cell suspensions separated by d. gradient centrifugation. Following this three

bands were formed on the gradients and the cell populations from these were characterized using periodic acid Schiff's (PAS) reactivity for mucosubstances, hemeatoxylin and eosin staining, and immunoreactivity with both monoclonal and polyclonal antibodies. The first band consisted of polygonal cells and other more minor cell types, the second cell band contained mainly polygonal and PAS-pos. goblet epithelial cells, while the third band consisted of mainly erythrocytes. There were significant differences in the eicosanoid generating potential of the isolated cells, with cells from the second band generating significantly more 12-HETE and 8,15-DiHETE than those from both the first band and unfractionated populations. The eicosanoid generating activity of the trout gill epithelial cell line, RTG-W1, was also elucidated. It proved to be a modest generator of eicosanoids in that only low levels of thromboxane B2 and prostaglandin E2 were detected while no lipoxygenase products were observed

IT **119433-37-3**
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence)
(eicosanoid generating capacity of isolated cell populations from the gills of rainbow trout)

RN 119433-37-3 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,14S,16Z,19Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 11 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:477973 HCAPLUS
DOCUMENT NUMBER: 129:202364
TITLE: N-3 fatty acid deficiency in the rat pineal gland: effects on phospholipid molecular species composition and endogenous levels of melatonin and lipoxygenase products
AUTHOR(S): Zhang, Hongjian; Hamilton, Jillonne H.; Salem, Norman, Jr.; Kim, Hee-Yong
CORPORATE SOURCE: Section of Mass Spectrometry, National Institute on Alcohol Abuse and Alcoholism, National Institutes of Health, Rockville, MD, 20852, USA
SOURCE: Journal of Lipid Research (1998), 39(7), 1397-1403
CODEN: JLPRAW; ISSN: 0022-2275
PUBLISHER: Lipid Research, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

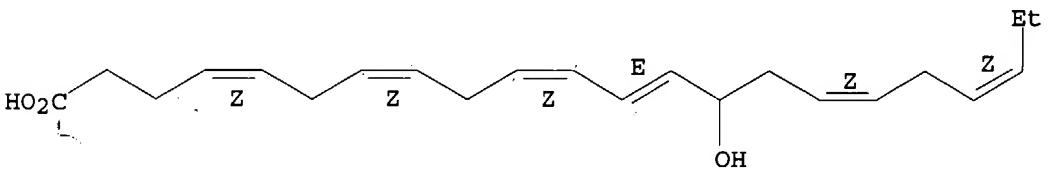
AB N-3 essential fatty acid deficiency affects a number of biol. and physiol. processes. In this study, the authors investigated the effect of n-3 essential fatty acid status on two key pineal biochem. functions, melatonin production and lipoxygenation, using pineal glands from rats given

an n-3-adequate or n-3-deficient diet. The pineal total lipid profile and phospholipid mol. species distribution altered by n-3 deficiency were evaluated in parallel. In pineal glands from n-3-deficient rats, an 87% reduction of 22:6n-3 (docosahexaenoic acid) was observed, and this decrease was accompanied by increases in 22:4n-6 (docosatetraenoic acid, 3-fold), 22:5n-6 (docosapentaenoic acid, 12-fold), and 20:4n-6 (arachidonic acid, 48%). The significant decrease of 22:6n-3 containing species in phosphatidylcholine (PC), phosphatidylethanolamine (PE), and phosphatidylserine (PS) was also evident. These decreases in 22:6n-3 containing PL species were compensated by substantial accumulations of 22:4n-6 or 22:5n-6 and slight increases in 20:4n-6 containing PL species in PC and PE. In PS, however, the accumulation of n-6 species was not adequate to compensate for the loss of 22:6n-3 species. N-3 deficiency significantly reduced non-esterified 20:4n-6 and 22:6n-3 levels in pineals (25% and 65%, resp.). Concomitantly, the endogenous 12-HETE level decreased by 35% in deficient pineals. In contrast, n-3 deficiency led to a more than 60% increase in the daytime pineal melatonin level. In conclusion, n-3 fatty acid deficiency not only has profound effects on pineal lipid profiles but also on pineal biochem. activities. These results suggest that n-3 fatty acids may play a critical role in regulating pineal function.

IT **87042-40-8 90780-52-2**
RL: BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)
(n-3 fatty acid deficiency in rat pineal gland effects on phospholipid mol. species composition and endogenous levels of melatonin and lipoxygenase products)

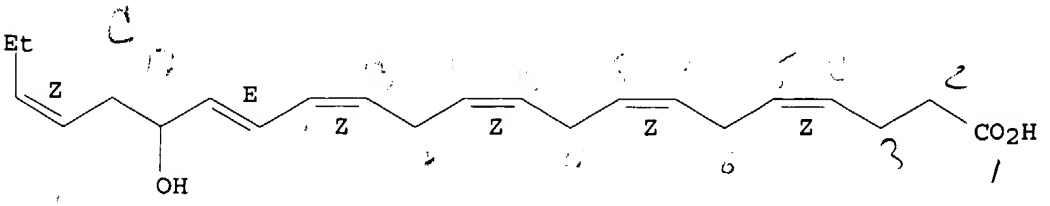
RN 87042-40-8 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 90780-52-2 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, (4Z,7Z,10Z,13Z,15E,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 12 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:157651 HCAPLUS
DOCUMENT NUMBER: 124:227170

TITLE: Production of monohydroxy derivatives from highly unsaturated fatty acids in the gills of red sea bream Pagrus major
AUTHOR(S): Iijima, Noriaki; Hada, Takahiko; Kayama, Mitsu
CORPORATE SOURCE: Faculty of Applied Biological Science, Hiroshima Univ., Hiroshima, 739, Japan
SOURCE: Fisheries Science (1996), 62(1), 114-21
CODEN: FSCIEH; ISSN: 0919-9268
PUBLISHER: Japanese Society of Fisheries Science
DOCUMENT TYPE: Journal
LANGUAGE: English

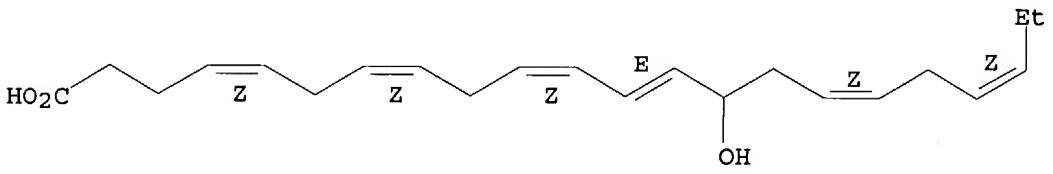
102(b)
Claim 29

AB 12-Hydroxyeicosatetraenoic acid and 15-hydroxyeicosatetraenoic acid were produced as major and minor monohydroxylated products in a microsome fraction, when [1-14C]arachidonic acid was incubated with the microsome or cytosol fraction prepared from frozen stored gill tissue of red sea bream P. major. The endogeneous products extracted from the microsome fraction of the red sea bream gill were isolated by HPLC and identified as 12-hydroxyeicosatetraenoic acid, 12-hydroxyeicosapentaenoic acid, and 14-hydroxydocosahexaenoic acid by UV absorption spectrometry and gas chromatog.-mass spectrometry. These data suggest that arachidonic acid, eicosapentaenoic acid, and docosahexaenoic acid are converted to their monohydroxy derivs. via the hydroperoxides by the action of 12-lipoxygenase-like enzyme, which is distributed in the microsomes of red sea bream gill.

IT **87042-40-8**
RL: BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)
(monohydroxy derivs. formation from highly unsatd. fatty acids in the gills of red sea bream)

RN 87042-40-8 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L28 ANSWER 13 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:939306 HCAPLUS
DOCUMENT NUMBER: 124:26230
TITLE: Biosynthesis of docosanoids by human platelet: Cardiovascular properties
AUTHOR(S): Karanian, John W.; Kim, Hee Yong; Salem, Norman Jr.
CORPORATE SOURCE: Laboratory Membrane Biochemistry and Biophysics, DICBR/NIAAA, Rockville, MD, 20852, USA
SOURCE: Cardiovascular Disease 2: Cellular and Molecular Mechanisms, Prevention, and Treatment, [Proceedings of the Washington International Spring Symposium], 14th, Washington, D. C., June 6-10, 1994 (1995), Meeting Date 1994, 269-77. Editor(s): Gallo, Linda L. Plenum: New York, N. Y.
CODEN: 61ZNA9
DOCUMENT TYPE: Conference

LANGUAGE: English

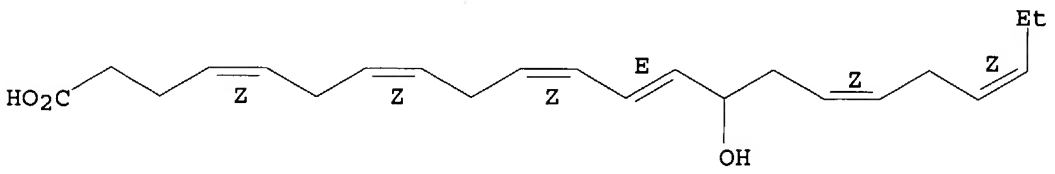
AB A reliable purification and quantification method is presented that was used to characterize the metabolism and production of the hydroxylated derivs. of 22:5n3, 22:6n3, 22:5n5 and 22:5n6 from mammalian platelets. Their biol. properties in platelet and vascular smooth muscle cell function is discussed.

IT **87042-40-8 90780-52-2**
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative); PROC (Process)
(biosynthesis and metabolism of docosanoids by human platelets and their cardiovascular properties)

RN 87042-40-8 HCAPLUS

CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)-(9CI) (CA INDEX NAME)

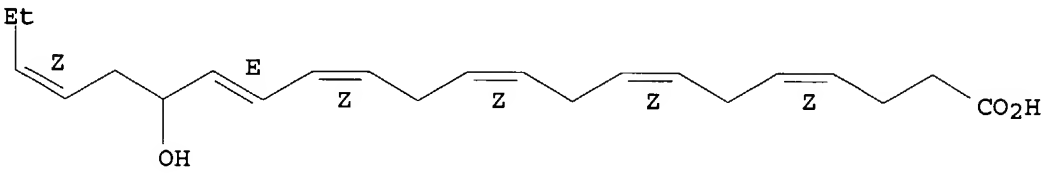
Double bond geometry as shown.



RN 90780-52-2 HCAPLUS

CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, (4Z,7Z,10Z,13Z,15E,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



L28 ANSWER 14 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1995:568335 HCAPLUS

DOCUMENT NUMBER: 122:311127

TITLE: Eicosanoid generating capacities of different tissues from the rainbow trout, Oncorhynchus mykiss

AUTHOR(S): Knight, John; Holland, Jason W.; Bowden, Linda A.; Halliday, Katrina; Rowley, Andrew F.

CORPORATE SOURCE: School Biological Sciences, University Wales, Swansea, Singleton Park, SA2 8PP, UK

SOURCE: Lipids (1995), 30(5), 451-8
CODEN: LPDSAP; ISSN: 0024-4201

PUBLISHER: AOCS Press

DOCUMENT TYPE: Journal

LANGUAGE: English

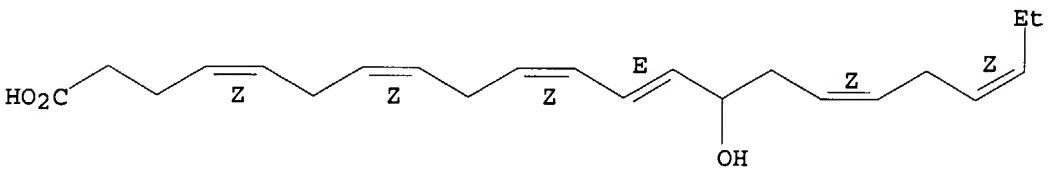
AB The eicosanoid-generating potential of the brain, gills, skin, ovary, muscle, eye, liver, spleen, heart, and alimentary canal in the rainbow trout, O. mykiss, was examined All the organs/tissues examined synthesized the 12-lipoxygenase products, 12-hydroxyeicosatetraenoic acid (12-HETE),

and 12-hydroxyeicosapentaenoic acid (12-HEPE), implying the widespread nature of this enzyme in trout. Both prostaglandin E and LTC were also found in variable amts. in the organs, with the greatest amount of PGE found in the gill. Leukotriene (LT) B4 and LTB5 were found in supernatants from Ca2+ ionophore-challenged brain, skin, ovary, liver, spleen, and heart, but the lipoxins A4 and A5 were only present in brain, ovary, and spleen in relatively small amts. As lipoxins have previously been shown to be synthesized by macrophages in rainbow trout, and related cells (microglial cells) are found in the brain of mammals, the localization of macrophage-like cells in trout brain was investigated immunocytochem. Monoclonal antibodies specific for trout leukocytes failed to identify any microglial-like cells in sections of the brain, although microvessels containing immuno-pos. reaction products were observed A number of distinct lipoxygenase products were found in supernatants of ionophore-challenged gill, including 14-hydroxydocosahexaenoic acid, 12-HETE, and 12-HEPE, and a large number of dihydroxy fatty acid derivs. with conjugated triene chromophores. One of these products was tentatively identified as 8(R),15(S)-dihydroxyeicosatetraenoic acid, a dual 12- and 15-lipoxygenase product, but apparently no LTB4 was generated by this tissue.

IT **87042-40-8**
RL: BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)
(eicosanoid formation by organs of rainbow trout)

RN 87042-40-8 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



L28 ANSWER 15 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1994:677471 HCAPLUS
DOCUMENT NUMBER: 121:277471
TITLE: Inhibitory effects of n-6 and n-3 hydroxy fatty acids on thromboxane (U46619)-induced smooth muscle contraction
AUTHOR(S): Karanian, J. W.; Kim, H. Y.; Salem, Norman, Jr.
CORPORATE SOURCE: Lab. Membrane Biochem. and Biophysics, Natl. Inst. Alcohol Abuse and Alcoholism, Bethesda, MD, USA
SOURCE: Journal of Pharmacology and Experimental Therapeutics (1994), 270(3), 1105-9
CODEN: JPETAB; ISSN: 0022-3565
DOCUMENT TYPE: Journal
LANGUAGE: English

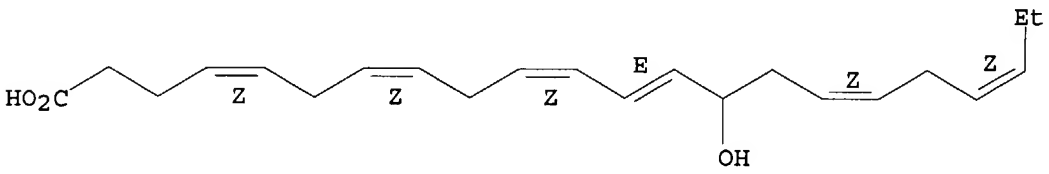
AB Mammalian platelets are capable of enzymically producing a number of n-6 and n-3 hydroxy fatty acids. Human platelet suspensions produce two major docosahexaenoic acid (22:6n3) metabolites, namely, 11-OH- and 14-OH-22:6n3. The hydroxy fatty acids which were formed by human platelets and purified by high performance liquid chromatog. specifically antagonize the contractile effects of a thromboxane mimetic, U46619, in airway, visceral and, especially, in the vascular smooth muscle prepns. studied.

The efficacy of OH-22:6n3 (IC25 = 1.1 μM) was compared to other n-6 and n-3 hydroxy fatty acids in the rat aortic ring preparation The OH-22:6n3 was significantly more potent with the exception of OH-22:5n3. The rank order of their potency was 14-OH-22:5n3 ≥ 14-OH-22:6n3 > 17-OH-22:6n3 ≥ 11-OH-22:6n3 ≥ 11-OH-22:5n3 > 12-OH-20:5n3 ≥ 12-OH-20:4n6 ≥ 14-OH-22:5n6 > 13-OH-18:2n6 > 14-OH-22:5n5. Antagonism of thromboxane effects may be an important aspect of the biol. function of 22-carbon n-3 hydroxylated fatty acids in the platelet-vascular smooth muscle cell interactions.

IT **87042-40-8 90780-52-2**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(n-3 and n-6 hydroxy fatty acid inhibition of thromboxane (U46619)-induced smooth muscle contraction)

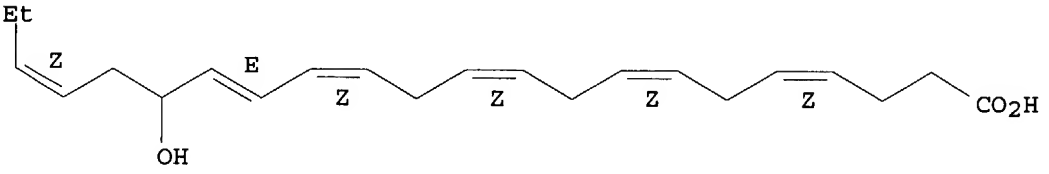
RN 87042-40-8 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 90780-52-2 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, (4Z,7Z,10Z,13Z,15E,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



L28 ANSWER 16 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1994:598954 HCAPLUS
DOCUMENT NUMBER: 121:198954
TITLE: Conformational analysis of isolated docosahexaenoic acid (22:6 n-3) and its 14 (S) and 11 (S) hydroxy derivatives by force field calculations
AUTHOR(S): Albrand, Michel; Pageaux, Jean-Francois; Lagarde, Michel; Dolmazon, Rene
CORPORATE SOURCE: Service de Chimie Organique, B 403, Institut National des Sciences Appliquees, 20 Avenue Albert Einstein, Villeurbanne, 69621, Fr.
SOURCE: Chemistry and Physics of Lipids (1994), 72(1), 7-17
CODEN: CPLIA4; ISSN: 0009-3084
DOCUMENT TYPE: Journal
LANGUAGE: English

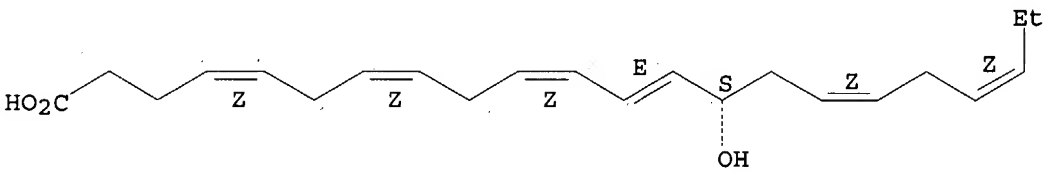
AB Docosahexaenoic acid (DHA) and two of its lipoxygenase end-products, the 11- and 14-hydroxy derivs., of biol. relevance were studied for their

privileged conformations using mol. mechanics. As an isolated mol., DHA adopted helical conformations. However, a more extended helical conformation would fit better with the hydrophobic interactions expected with DHA esterified within glycerophospholipids. The most stable conformations of the hydroxy derivs. of DHA appeared as coiled ones where an intramol. hydrogen bond occurs between the carboxylic and the hydroxy groups. Among the latter conformations, one for each hydroxy derivative would fit better with the requirement of the largest distance between the hydrophobic and hydrophilic centers within the mol. for being inserted in membrane phospholipids where the hydroxy derivs. are likely to be located in their unesterified form. As thromboxane A2 (TXA2) antagonist, DHA and its hydroxy derivs. were compared with minimized conformations of TXA2 and one of its potent antagonist recently described, (R)-(+)-TCV-144. Interestingly, the 14- hydroxy derivative of DHA, previously reported as the most potent TXA2 antagonist among the DHA derivs., exhibited stable conformations quite similar to those of TXA2 and (R)-(+)-TCV-144.

IT **119433-37-3**
RL: PRP (Properties)
(conformational anal. of docosahexaenoic acid and two hydroxy derivs. by force field calcns.)

RN 119433-37-3 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,14S,16Z,19Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L28 ANSWER 17 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1994:478737 HCAPLUS
DOCUMENT NUMBER: 121:78737
TITLE: Polyunsaturated-fatty-acid oxidation in Hydra: regioselectivity, substrate-dependent enantioselectivity and possible biological role
AUTHOR(S): Di Marzo, Vincenzo; Gianfrani, Carmen; De Petrocellis, Luciano; Milone, Alfredo; Cimino, Guido
CORPORATE SOURCE: Ist. Chim. Mol. Interesse Biol., CNR, Arco Felice, 80072, Italy
SOURCE: Biochemical Journal (1994), 300(2), 501-7
CODEN: BIJOAK; ISSN: 0264-6021
DOCUMENT TYPE: Journal
LANGUAGE: English

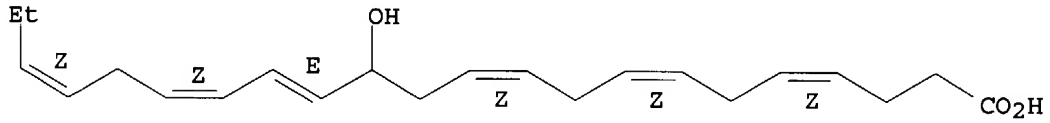
AB A novel and abundant lipoxygenase-like activity converting cis-eicosa-5,8,11,14-tetraenoic acid (arachidonic acid) into (11R)-hydroxyeicosatetraenoic acid has been recently described in homogenates of the freshwater hydrozoan Hydra vulgaris. In this study, other substrates for this enzyme were selected from the polyunsatd. fatty acids (PUFAs) present in H. vulgaris, and the chemical natures of the hydroperoxy and hydroxy derivs. produced, as well as the activity of some of the latter on hydroid tentacle regeneration, were investigated. The highest conversion among C20 fatty acids was observed for arachidonic acid, and among C18 fatty acids for cis-octadeca-9,12,15- and

cis-octadeca-6,9,12-trienoic (α- and γ-linolenic) acids. Cis double bonds on the 10th C atom from the aliphatic end of the substrate (e.g. C-9, C-11, and C-13 resp. in C18, C20, and C22 PUFAs) were regiospecifically peroxidized. Conversely, trans-octadeca-9,12-dienoic (linelaidic) acid was not a substrate for lipoxygenase activity. Enantioselectivity of lipoxygenation depended on the degree of unsatn. of the substrate, with the amount of the R enantiomer increasing when passing, for example, from cis-eicosa-11,14-dienoic to cis-eicosa-5,8,11,14,17-pentaenoic acid. Regiospecific formation of keto acids was observed only when incubating C18 PUFAs. Com. available hydroxyacids corresponding to the reaction products of some of the most abundant H. vulgaris PUFAs were tested for effects on Hydra tentacle regeneration. An enhancement of average tentacle number, in a fashion depending on the stereochem. and on the number of double bonds, was found for 2 compds., thus suggesting for the 11-lipoxygenase-like enzyme a role in the production of metabolites potentially active in the control of hydroid regenerative processes.

IT **90780-53-3 121695-00-9**
RL: FORM (Formation, nonpreparative)
(formation of, by lipoxygenase of hydra)

RN 90780-53-3 HCAPLUS
CN 4,7,10,14,16,19-Docosahexaenoic acid, 13-hydroxy-, (4Z,7Z,10Z,14E,16Z,19Z)- (9CI) (CA INDEX NAME)

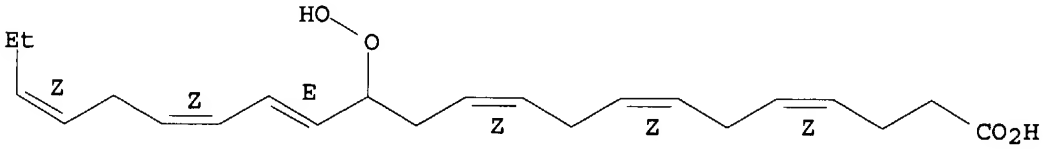
Double bond geometry as shown.



Claim 28
102.b.

RN 121695-00-9 HCAPLUS
CN 4,7,10,14,16,19-Docosahexaenoic acid, 13-hydroperoxy-, (E,Z,Z,Z,Z,Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L28 ANSWER 18 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:	1994:473909 HCAPLUS
DOCUMENT NUMBER:	121:73909
TITLE:	Antipsychotics containing docosahexaenoic acid or its derivatives
INVENTOR(S):	Nishikawa, Masazumi; Kimura, Seiji
PATENT ASSIGNEE(S):	Maruha Kk, Japan
SOURCE:	Jpn. Kokai Tokkyo Koho, 5 pp. CODEN: JKXXAF
DOCUMENT TYPE:	Patent
LANGUAGE:	Japanese
FAMILY ACC. NUM. COUNT:	1
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

JP 06072868	A2	19940315	JP 1992-227510	19920826
US 6306907	B1	20011023	US 1993-111831	19930825
PRIORITY APPLN. INFO.:			JP 1992-227510 A	19920826

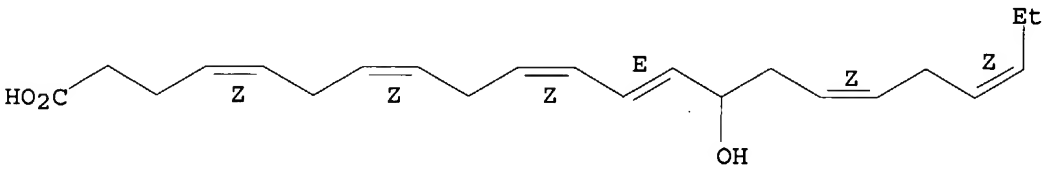
AB Antipsychotics contain ≥1 compds. chosen from docosahexaenoic acid (I) or its derivs. as active ingredients, which show high safety and are useful for prevention and treatment of psychosis. I at 30 μM reduced N-methyl-D-aspartic acid receptor antagonism of phencyclidine in hippocampus CA1 region nerve cell sample of sliced rat brain. Et docosahexaenoate at 300 mg 3 times a day improved neg. symptoms in schizophrenia patients and showed no side effects.

IT **87042-40-8**
RL: BIOL (Biological study)
(as antipsychotic)

RN 87042-40-8 HCAPLUS

CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



1, 29
10261

L28 ANSWER 19 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:	1994:431729 HCAPLUS
DOCUMENT NUMBER:	121:31729
TITLE:	Lipoxygenation of docosahexaenoic acid by the rat pineal body
AUTHOR(S):	Sawazaki, Shigeki; Salem, Norman, Jr.; Kim, Hee-Yong
CORPORATE SOURCE:	Lab. Membrane Biochem. Biophys., Natl. Inst. Alcohol Abuse and Alcoholism, Bethesda, MD, USA
SOURCE:	Journal of Neurochemistry (1994), 62(6), 2437-47 CODEN: JONRA9; ISSN: 0022-3042
DOCUMENT TYPE:	Journal
LANGUAGE:	English

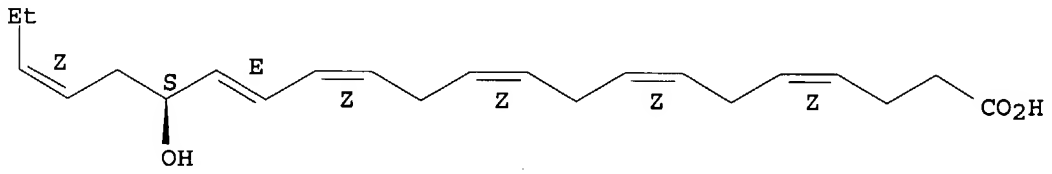
AB Based on the inhibitor profile, production rate, and stereochem. purity of the hydroxylated products, it was demonstrated that lipoxygenation in rat brain occurs only in the pineal. Both positional and stereochem. specificities of the hydroxylation were observed only in pineal, clearly indicating that only the pineal is capable of lipoxygenating polyunsatd. fatty acids among the rat brain regions examined Cerebral cortex also produced hydroxy products; however, they were racemic mixts., indicating the peroxidn. was responsible for their production Rat pineal homogenate, obtained after the brain was perfused, metabolized [14C]docosahexaenoic acid ([1-14C]22:6n3) to monohydroxy derivs., primarily by the 12- and, to a lesser extent, by the 15-lipoxygenase (LO) reaction. The resulting metabolites were 14(S)- and 17(S)-hydroxydocosahexaenoic acid (HDoHE), as determined by reversed-phase HPLC, chiral-phase HPLC, thermospray liquid chromatog.-mass spectrometry, and gas chromatog.-mass spectrometry. Because blood was removed by perfusion of the brain before incubation, it was clear that the observed LO activity was not due to contamination with blood cell components. The production rate of 17-HDoHE from 22:6n3 was higher than that of 15-hydroxyperoxy-1,8,11,13-eicosatetraenoic acid from 20:4n6, whereas 12-LO activity toward these two substrates was comparable. These

monohydroxy metabolites were also detected in the pineal body lipid extract using neg. ion chemical ionization mass spectrometry. This is the first observation of endogenous production of hydroxylated compds. in pineal. The ratio of endogenous 15-LO to 12-LO products was considerably higher than that of the in vitro production from exogenous substrate. In some cases, 15-LO products were the major LO metabolites present in the lipid extract of pineal body for both 20:4n6 and 22:6n3. Both 12- and 15-LO activities were recovered mainly in the microsomal plus cytosolic fraction. In addition to monohydroxy products, epoxy, hydroxy derivs. were formed from 22:6n3 by the pineal. The major isomer was identified as 12-hydroxy-13,14-epoxy-22:5n3.

IT **92693-03-3 119433-37-3 155976-52-6**
155976-53-7
RL: FORM (Formation, nonpreparative)
(formation of, from docosahexaenoate by pineal gland, lipoxygenase in)

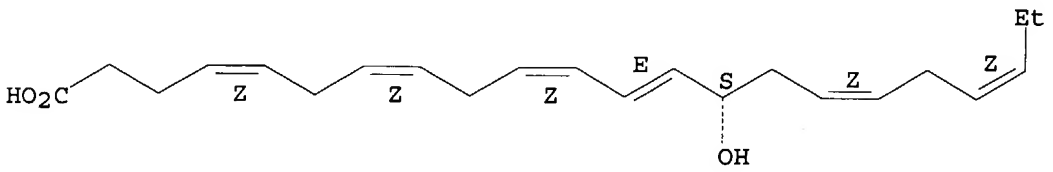
RN 92693-03-3 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, [S-(E,Z,Z,Z,Z,Z)]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



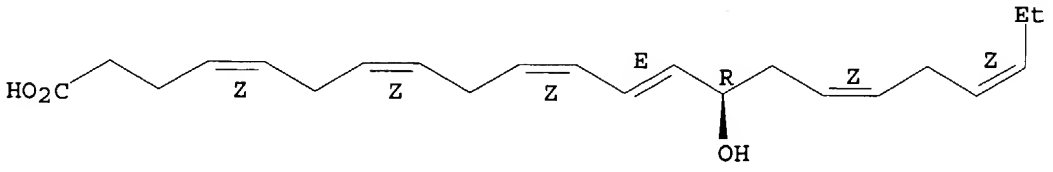
RN 119433-37-3 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,14S,16Z,19Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



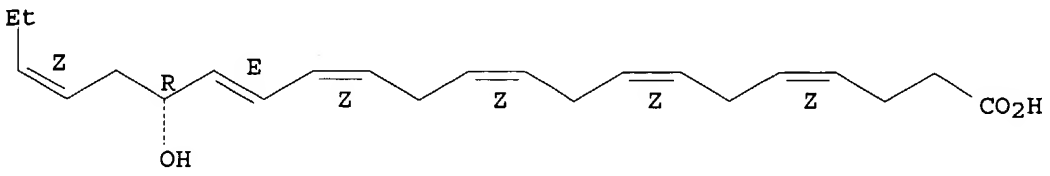
RN 155976-52-6 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, [R-(E,Z,Z,Z,Z,Z)]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 155976-53-7 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, (4Z,7Z,10Z,13Z,15E,17R,19Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L28 ANSWER 20 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1994:265249 HCAPLUS
DOCUMENT NUMBER: 120:265249
TITLE: High-performance liquid chromatography-thermospray mass spectrometry of epoxy polyunsaturated fatty acids and epoxyhydroxy polyunsaturated fatty acids from an incubation mixture of rat tissue homogenate
AUTHOR(S): Yamane, Mototeru; Abe, Akihisa; Yamane, Sayoko
CORPORATE SOURCE: Dep. Biochem., Tokyo Med. Coll., Tokyo, Japan
SOURCE: Journal of Chromatography, B: Biomedical Sciences and Applications (1994), 652(2), 123-36
CODEN: JCBBEP; ISSN: 1387-2273
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A method for the anal. of epoxy polyunsatd. fatty acids (EpPUFAs) and epoxyhydroxy polyunsatd. fatty acids (EpHPUFAs) in rat tissue homogenate, with homo-γ-linolenic acid (20:3,n-6), arachidonic acid (20:4,n-6), eicosapentaenoic acid (20:5,n-3) or docosahexaenoic acid (22:6,n-3) as a substrate, was developed. Extraction with dichloromethane at pH 4-5 and concentration in the presence of pyridine were performed. Spectral anal. of chromatograms obtained with HPLC-thermospray mass spectrometry showed the presence of EpPUFAs, EpHPUFAs and dihydroxy metabolites (DiHPUFAs) of EpPUFAs corresponding to each precursor fatty acid. On a selected-ion monitoring chromatogram, many EpPUFAs, EpHPUFAs and DiHPUFAs in an extract from an incubation mixture of each precursor fatty acid in aged rat tissue homogenate were detected simultaneously within 70 min. EpPUFAs and DiHPUFAs derived from 20:3 (n-6) or 20:5 (n-3) were detected in significant amts. From these results, a highly active cytochrome P 450 system or nonenzymic oxidative reactions in aged rat tissue homogenate were suggested.

IT **87042-40-8 90780-52-2 90906-41-5**
RL: ANT (Analyte); ANST (Analytical study)
(detection of, in animal tissue by HPLC with thermospray mass spectrometry)

RN 87042-40-8 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

10261

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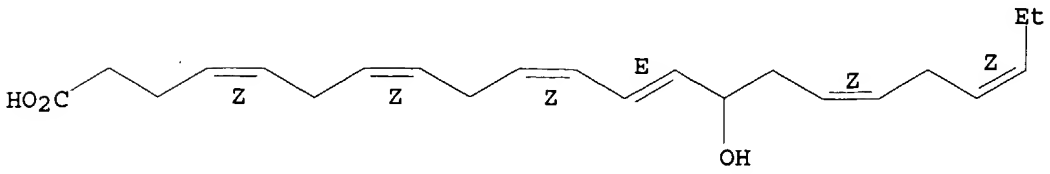
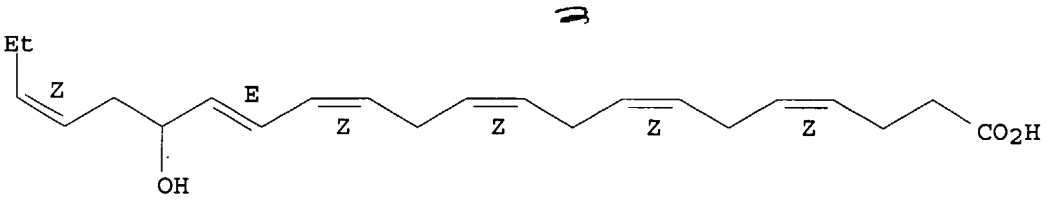


29

RN 90780-52-2 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, (4Z,7Z,10Z,13Z,15E,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



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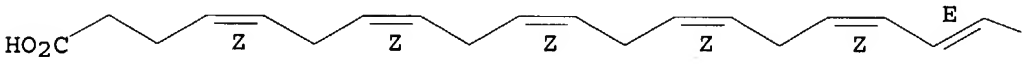
RN 90906-41-5 HCAPLUS
CN 4,7,10,13,16,18-Docosahexaenoic acid, 20-hydroxy-, (4Z,7Z,10Z,13Z,16Z,18E)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



102(b)

PAGE 1-B

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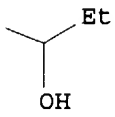


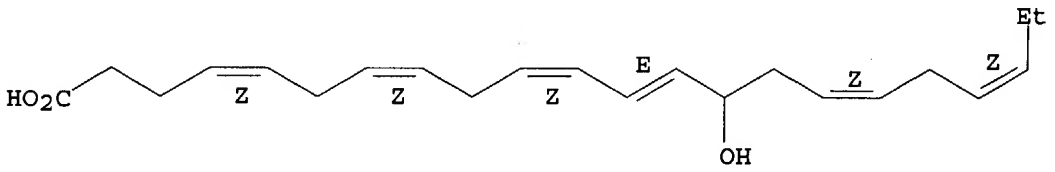
L28 ANSWER 21 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1994:7455 HCAPLUS
DOCUMENT NUMBER: 120:7455
TITLE: Effect of diets rich in linoleic or α-linolenic acid on phospholipid fatty acid composition and eicosanoid production in Atlantic salmon (Salmo salar)
AUTHOR(S): Bell, J. Gordon; Dick, James R.; Sargent, John R.
CORPORATE SOURCE: Sch. Nat. Sci., Univ. Stirling, Stirling, FK9 4LA, UK
SOURCE: Lipids (1993), 28(9), 819-26
CODEN: LPDSAP; ISSN: 0024-4201
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Atlantic salmon post-smolts were fed diets rich in linoleic acid (sunflower oil, SO), α-linolenic acid (linseed oil, LO) or long-chain polyunsatd. fatty acids (fish oil, FO) for a period of 12 wk.

In the liver phospholipids of fish fed SO, the levels of 18:2n-6, 20:2n-6 and 20:4n-6 were significantly elevated compared to both other treatments. In choline phospholipids (CPL), ethanolamine phospholipids (EPL) and phosphatidylserine (PS) the levels of 22:4n-6 and 22:5n-6 were significantly elevated in fish fed SO. In liver phospholipids from fish fed LO, 18:2n-6, 20:2n-6 and 20:3n-6 were significantly elevated but 20:4n-6, 22:4n-6 and 22:5n-6 were similar or significantly decreased compared to fish fed FO. Liver phospholipids from fish fed LO had increased 18:3n-3 and 20:4n-3 compared to both other treatments while EPL and phosphatidylinositol (PI) also had increased 20:5n-3. In fish fed LO, 22:6n-3 was significantly reduced in CPL, PS and PI compared to fish fed FO. Broadly similar changes occurred in gill phospholipids. Production of 12-lipoxygenase metabolites in isolated gill cells stimulated with the Ca2+-ionophore A23187 were significantly reduced in fish fed either SO or LO compared to those fed FO. However, the ratio 12-hydroxy-5,8,10,14-eicosatetraenoic acid (12-HETE)/12-hydroxy-5,8,10,14,17-eicosapentaenoic acid (12-HEPE) was significantly elevated in stimulated gill cells from SO-fed fish. Although mean values of thromboxane B2 (TXB2) and prostaglandin E2 (PGE2) were increased in fish fed SO, they were not significantly different from those of the other two treatments.

IT **87042-40-8**
RL: BIOL (Biological study)
(of gill of salmon, dietary linoleic and linolenic acids effect on)

RN 87042-40-8 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



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L28 ANSWER 22 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1993:665901 HCAPLUS
DOCUMENT NUMBER: 119:265901
TITLE: Facile preparation and structural determination of monohydroxy derivatives of docosahexaenoic acid (HDoHE) by α-tocopherol-directed autoxidation
AUTHOR(S): Reynaud, Denis; Thickitt, Christopher P.; Pace-Asciak, Cecil R.
CORPORATE SOURCE: Res. Inst., Hosp. Sick Child., Toronto, ON, M5G 1X8, Can.
SOURCE: Analytical Biochemistry (1993), 214(1), 165-70
CODEN: ANBCA2; ISSN: 0003-2697
DOCUMENT TYPE: Journal
LANGUAGE: English

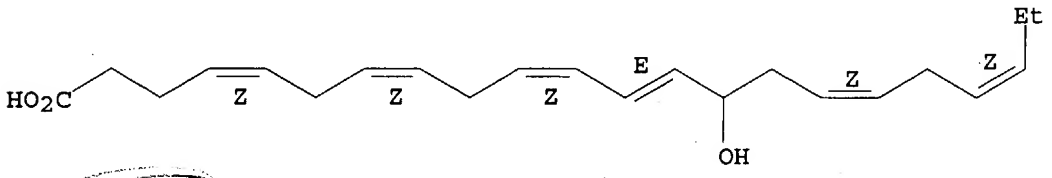
AB Polyunsatd. fatty acids are oxidized through both enzymic and nonenzymic reactions into hydroxy derivs. With increasing interest in dietary manipulations through ingestion of the highly unsatd. fish oil fatty acids, eicosapentaenoic acid and docosahexaenoic acid (DHA), methods to measure their metabolism are required. In this study the authors report the simple and expedient α-tocopherol-directed autoxidative preparation of a series of monohydroxy derivs. of DHA to provide a relatively homogeneous hydroxylation along each of the double bonds of the fatty substrate.

Products were purified by high-performance liquid chromatog. (HPLC) and their structures elucidated by the characteristic fragmentation pattern of the hydrogenated Me ester trimethylsilyl ether derivs. by gas chromatog.-mass spectrometry. Nine products were isolated in 20.2% yield overall, ranging from 1.55 to 4.14% yield of isolated compound These were identified as 7, 8, 10, 11, 13, 14, 16, 17, and 20-HDoHEs (monohydroxydocosahexaenoic acids). Two of these products (14- and 17-HDoHE) could not be separated under the HPLC conditions used but were clearly distinguished using selected ion chromatog. by their distinct mass spectral fragmentation. This method is highly suitable for the generation of stds. to investigate the metabolism of DHA in tissues.

IT **87042-40-8 90780-51-1 90780-52-2**
90780-53-3 90906-41-5
RL: FORM (Formation, nonpreparative)
(formation of, by docosahexaenoate tocopherol-directed autoxidn., structural characterization in relation to)

RN 87042-40-8 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)-(9CI) (CA INDEX NAME)

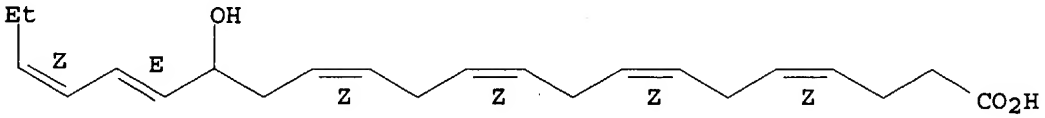
Double bond geometry as shown.



(29) 102(b)

RN 90780-51-1 HCAPLUS
CN 4,7,10,13,17,19-Docosahexaenoic acid, 16-hydroxy-, (4Z,7Z,10Z,13Z,17E,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.

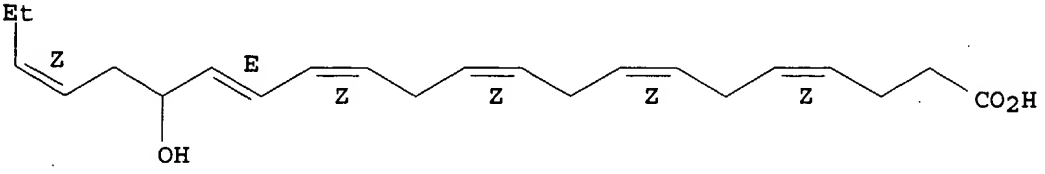


Claim 32 102(b)

RN 90780-52-2 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, (4Z,7Z,10Z,13Z,15E,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.

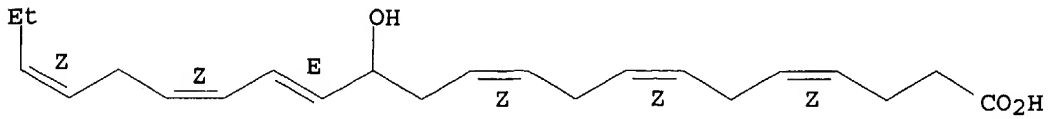
Claim 30



RN 90780-53-3 HCAPLUS
CN 4,7,10,14,16,19-Docosahexaenoic acid, 13-hydroxy-, (4Z,7Z,10Z,14E,16Z,19Z)-(9CI) (CA INDEX NAME)

Claim 28 102(b)

Double bond geometry as shown.



RN 90906-41-5 HCAPLUS
CN 4,7,10,13,16,18-Docosahexaenoic acid, 20-hydroxy-, (4Z,7Z,10Z,13Z,16Z,18E)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.

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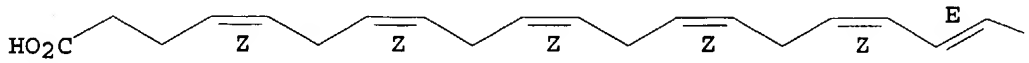
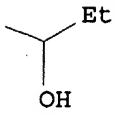
PAGE 1-A



PAGE 1-B



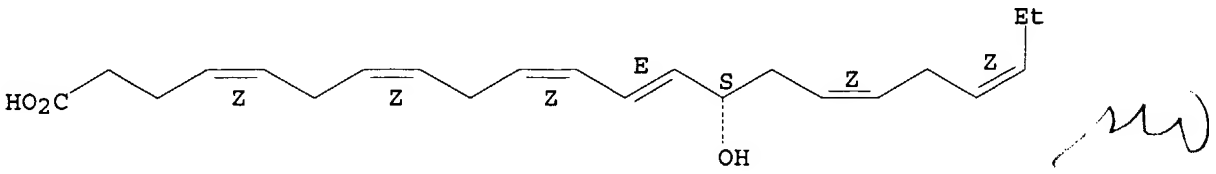
L28 ANSWER 23 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1993:467181 HCAPLUS
DOCUMENT NUMBER: 119:67181
TITLE: Structural analysis of hydroxy fatty acids by thermospray liquid chromatography/tandem mass spectrometry
AUTHOR(S): Kim, H. Y.; Sawazaki, S.
CORPORATE SOURCE: DICBR, NIAAA, Bethesda, MD, 20892, USA
SOURCE: Biological Mass Spectrometry (1993), 22(5), 302-10
CODEN: BIMSEH; ISSN: 1052-9306
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Thermospray liquid chromatog./tandem mass spectrometry provides a sensitive and convenient technique for the structural anal. of oxygenated polyunsaturates. Anal. of pentafluorobenzyl derivs. in the neg. ion mode under the filament- or discharge-on condition generated abundant [M - PFB]- ions. These ions were further fragmented by collision with argon and detected in the neg. ion mode. The neg. ion fragmentation pattern was examined for various oxygenated polyunsatd. fatty acid stds. as well as their deuterated and/or hydrogenated forms. Characteristic fragmentation occurs at the oxygenated C-C bonds, allowing unambiguous determination of the sites of oxygenation. The sample amount required is typically in the low tens of nanogram range. Using this method the structures of epoxy, hydroxy derivs. of 4,7,10,13,16,19-docosahexenoic acid (22:6w3) formed by soybean lipoxygenase were determined They were 13-hydroxy-16,17-epoxy-22:5w3 and 15-hydroxy-16,17-epoxy-22:5w3.

IT **119433-37-3**
RL: ANT (Analyte); ANST (Analytical study)
(determination of, by thermospray liquid chromatog and tandem mass spectrometry)

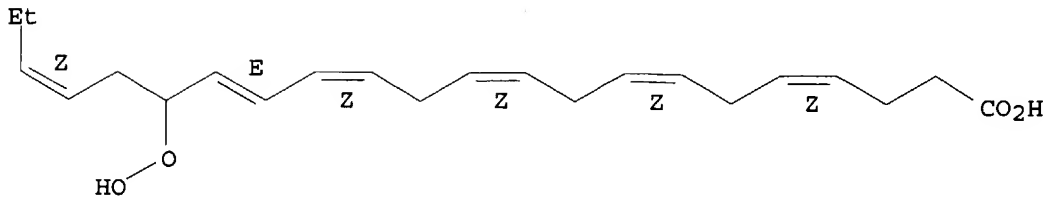
RN 119433-37-3 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,14S,16Z,19Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



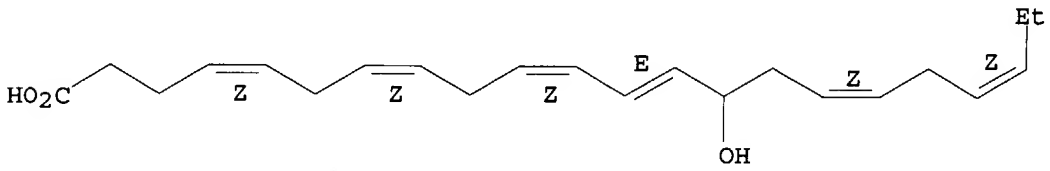
L28 ANSWER 24 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1992:587518 HCAPLUS
DOCUMENT NUMBER: 117:187518
TITLE: High-performance liquid chromatography-thermospray mass spectrometry of hydroperoxy polyunsaturated fatty acid acetyl derivatives
AUTHOR(S): Yamane, Mototeru; Abe, Akihisa; Yamane, Sayoko; Ishikawa, Fumio
CORPORATE SOURCE: Dep. Biochem., Tokyo Med. Coll., Tokyo, Japan
SOURCE: Journal of Chromatography (1992), 579(1), 25-36
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A method for the anal. of hydroperoxy polyunsatd. fatty acids was developed. The hydroperoxy groups were acetylated by acetic anhydride, and the mixture was partially purified on a Sep-Pak C18 cartridge and analyzed by high-performance liquid chromatog. with thermospray mass spectrometry. Generally, the base ion, [M + H - n(60)]+ or [M + H - n(60) - n(H2O)]+, is produced through elimination of acetic acid or water (n = number of hydroperoxy groups). The detection limit for these derivs. was approx. 1 pmol at concns. of hydroperoxy polyenoic acids prior to derivatization. Using this method, many hydroxy and hydroperoxy polyunsatd. fatty acid derivs. could be detected simultaneously within 30 min on a selected-ion monitoring detection chromatogram without a gradient system. The assay was successfully applied to hydroxy and hydroperoxy polyunsatd. fatty acids from an incubation mixture of rat brain homogenate to which polyunsatd. fatty acids has been added.
IT **70596-95-1 87042-40-8 90780-51-1 90780-52-2**
RL: ANT (Analyte); ANST (Analytical study)
(anal. of, by HPLC-mass spectrometry)
RN 70596-95-1 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroperoxy-, (4Z,7Z,10Z,13Z,15E,19Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



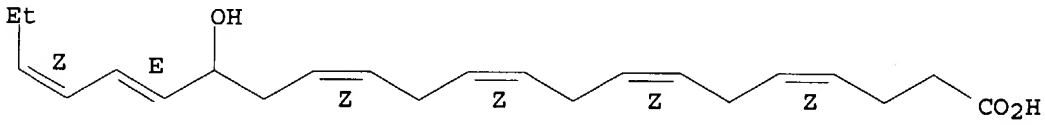
RN 87042-40-8 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



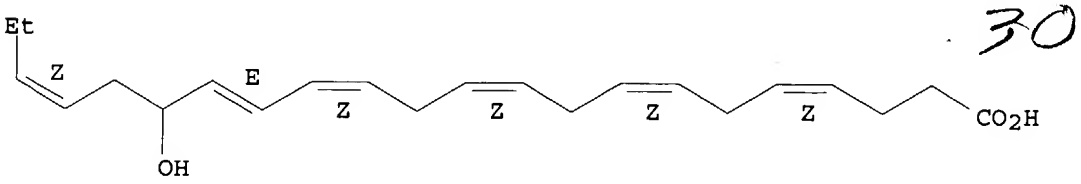
RN 90780-51-1 HCAPLUS
CN 4,7,10,13,17,19-Docosahexaenoic acid, 16-hydroxy-, (4Z,7Z,10Z,13Z,17E,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 90780-52-2 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, (4Z,7Z,10Z,13Z,15E,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



L28 ANSWER 25 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1992:530173 HCAPLUS
DOCUMENT NUMBER: 117:130173
TITLE: Analysis of hydroperoxides of eicosapentaenoic acid and docosahexaenoic acid from autoxidized squid viscera oil
AUTHOR(S): Chen, Jau Shyong; Hau, Lung Bin; Hwang, Lucy Sun
CORPORATE SOURCE: Dep. Food Sci. Nutr., Hung-Kuang Jr. Coll. Nurs. Med. Technol., Taichung, Taiwan

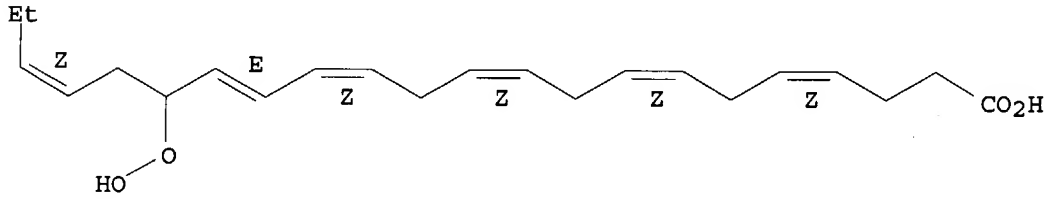
SOURCE: Zhongguo Nongye Huaxue Huizhi (1992), 30(1), 25-32
CODEN: CKNHAA; ISSN: 0578-1736
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

AB In order to evaluate the steric hindrance effect on autoxidn., hydroperoxides formed from squid (Martialia hyagesi) viscera oil and its fatty acid Me esters in the initial stage of autoxidn. (POV = 13.6 and 9.6, resp.) were analyzed by GC and GC-MS. The hydroperoxy groups of the EPA and DHA hydroperoxides from squid viscera oil were preferentially localized near the Me end of the mols. On the other hand, the hydroperoxy group of the EPA and DHA hydroperoxides from the squid viscera oil fatty acid Me esters were evenly distributed in the mols.

IT **70596-95-1 121694-99-3 121695-00-9**
121695-01-0
RL: FORM (Formation, nonpreparative)
(formation of, in squid viscera oil autoxidn.)

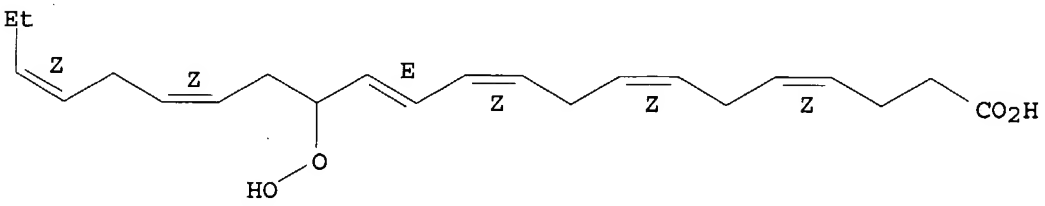
RN 70596-95-1 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroperoxy-, (4Z,7Z,10Z,13Z,15E,19Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



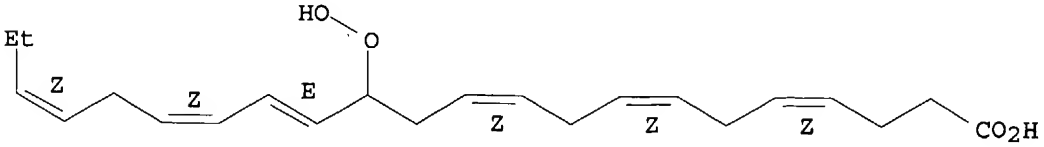
RN 121694-99-3 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroperoxy-, (E,Z,Z,Z,Z,Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 121695-00-9 HCAPLUS
CN 4,7,10,14,16,19-Docosahexaenoic acid, 13-hydroperoxy-, (E,Z,Z,Z,Z,Z)- (9CI) (CA INDEX NAME)

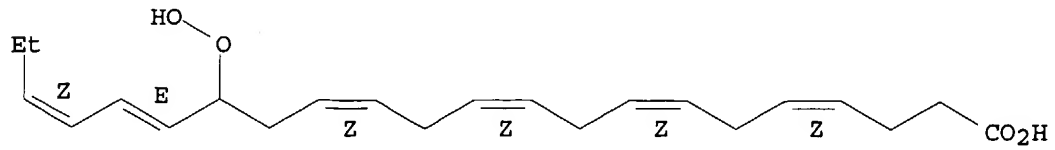
Double bond geometry as shown.



RN 121695-01-0 HCAPLUS

CN 4,7,10,13,17,19-Docosahexaenoic acid, 16-hydroperoxy-, (E,Z,Z,Z,Z,Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



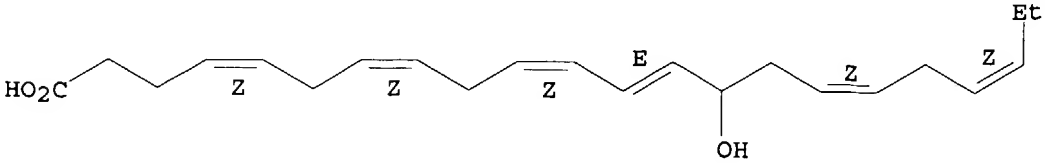
L28 ANSWER 26 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1992:234458 HCAPLUS
DOCUMENT NUMBER: 116:234458
TITLE: Effects of increasing dietary linoleic acid on phospholipid fatty acid composition and eicosanoid production in leukocytes and gill cells of Atlantic salmon (Salmo salar)
AUTHOR(S): Bell, J. G.; Sargent, J. R.; Raynard, R. S.
CORPORATE SOURCE: Sch. Nat. Sci., Univ. Stirling, Stirling, FK9 4LA, UK
SOURCE: Prostaglandins, Leukotrienes and Essential Fatty Acids (1992), 45(3), 197-206
CODEN: PLEAEU; ISSN: 0952-3278
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Diets containing linoleic acid at 10, 25, and 45% of total dietary fatty acids were fed to 3 groups of post-smolt Atlantic salmon for 18 wk. Incorporation of linoleic acid into membrane phospholipids of leukocytes and gills increased in response to dietary intake. In general, there was an increase in arachidonic acid and a decrease in eicosapentaenoic acid in the individual phospholipids of both cell types in response to increasing dietary linoleic acid. These changes in eicosanoid precursors were reflected in significantly increased plasma concns. of 6-keto-PGF1α and TXB2 in salmon given the highest dietary linoleic acid. In whole blood stimulated with the Ca ionophore A23187, LTB4, 12-HETE, and TXB2 were significantly increased and 12-HEPE significantly decreased in response to increasing dietary linoleic acid. In isolated gill cells stimulated with A23187, 12-HEPE, 12-HETE, 14-HDHE, and TXB2 were all decreased in response to increasing dietary linoleic acid, although the ratio of 12-HEPE/12-HETE was also decreased.

IT **87042-40-8**
RL: BIOL (Biological study)
(of blood, of Atlantic salmon, dietary linoleic acid effect on)

RN 87042-40-8 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



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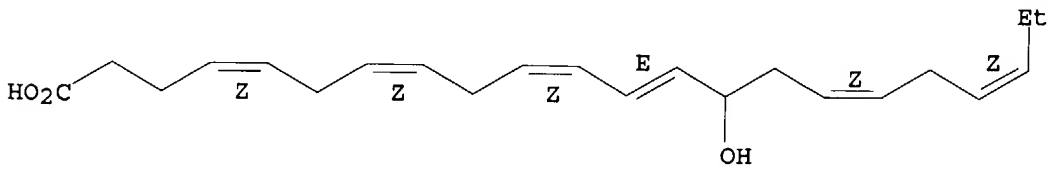
L28 ANSWER 27 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1992:211313 HCAPLUS
DOCUMENT NUMBER: 116:211313
TITLE: Identification and egg hatching activity of monohydroxy fatty acid eicosanoids in the barnacle Balanus balanoides
AUTHOR(S): Hill, E. M.; Holland, D. L.
CORPORATE SOURCE: Sch. Ocean Sci., Univ. Coll. North Wales, Anglesey, LL59 5EY, UK
SOURCE: Proceedings of the Royal Society of London, Series B: Biological Sciences (1992), 247(1318), 41-6
CODEN: PRLBA4; ISSN: 0080-4649
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Monohydroxy fatty acids (MHFAs) were isolated from homogenates of the barnacle B. balanoides and identified by gas chromatog.-mass spectrometry (GC-MS) as 14- and 17-hydroxy docosahexaenoic acids, 8-, 11-, 12-, 15- and 18-hydroxy eicosapentaenoic acids, 13- and 16-hydroxyoctadecatrienoic acids, and 9-, 13- and 15-hydroxyoctadecadienoic acids. Each monohydroxy fatty acid was tested for egg hatching activity in a bioassay using Elminius modestus egg masses, but 8-hydroxy-5, 9, 11, 14, 17-eicosapentaenoic acid (8-HEPE) was the only MHFA with barnacle egg hatching activity. Studies on the egg hatching activity of MHFAs prepared from the oxidation of polyunsatd. fatty acids showed that activity was confined to the 8-hdyroxy isomer of eicosapentaenoic acid and arachidonic acid, and that unsatn. at C5 and C14, but not C17, was essential for activity. In addition, the 8(R) conformation is necessary for activity, as 8(R)-HEPE caused egg hatching at 10-7M, whereas the enantiomer 8(S)-HEPE was inactive.

IT **87042-40-8 90780-52-2**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(in barnacle, identification and egg hatching activity of)

RN 87042-40-8 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



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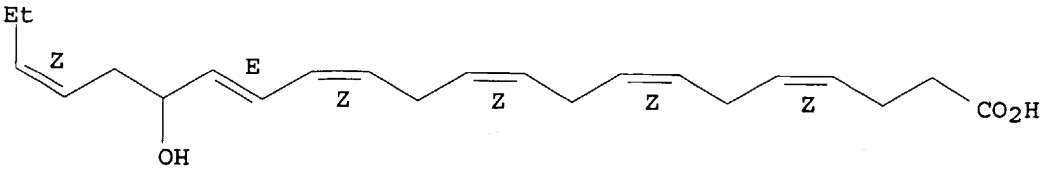
RN 90780-52-2 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, (4Z,7Z,10Z,13Z,15E,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



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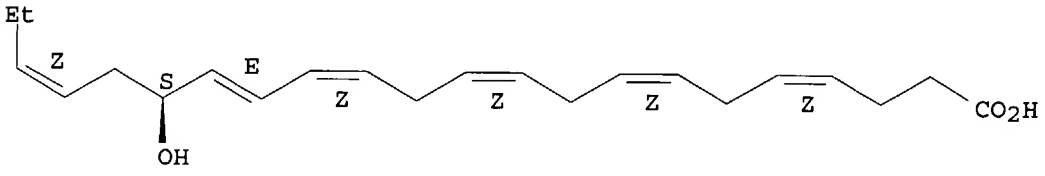
L28 ANSWER 28 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1992:171490 HCAPLUS
DOCUMENT NUMBER: 116:171490
TITLE: Detection of retinal lipid hydroperoxides in experimental uveitis
AUTHOR(S): Wu, Guey Shuang; Sevanian, Alex; Rao, Narsing A.
CORPORATE SOURCE: Sch. Med., Univ. South. California, Los Angeles, CA, USA
SOURCE: Free Radical Biology & Medicine (1992), 12(1), 19-27
CODEN: FRBMEH; ISSN: 0891-5849
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Phagocyte-mediated retinal lipid peroxidn. in exptl. uveitis i rats was studied using gas chromatog./mass spectrometry (GC/MS). Hydroperoxide-derived 10-, 11-, 13-, 14-, and 17-hydroxydocosahexaenoic acids (HDHE) were found in retinal membranes. Docosahexaenoic acid (22:6) was the major polyunsatd. fatty acid (PUFA) in photoreceptor membranes. Hydroperoxides from other retinal PUFA were found also. Arachidonic acid (20:4) yielded 8-, 9-, 11-, or 12-hydroxyeicosatetraenoic acid (HETE) as major products. Since 12-HETE could also arise from lipoxygenase-catalyzed oxygenation of free 20:4, the source of 12-HETE could be both peroxidative and lipoxygenase pathways. Peroxidative loss of 22:6 and accumulation of 20:4 were also noted. At the peak of inflammation, loss of 22:6 was close to 50% of the original amount while 20:4 increased more than 2-fold. The oxygen radicals derived from phagocytes initiate the retinal lipid peroxidn. The resultant formation of hydroperoxides, oxidative loss of 22:6, and accumulation of 20:4 appear to serve as amplification factors in subsequent biochem. events, such as polymorphonuclear chemotaxis and activation of cyclooxygenase.

IT **92693-03-3 119433-37-3 139974-01-9**
RL: BIOL (Biological study)
(of eye retina, in uveitis)

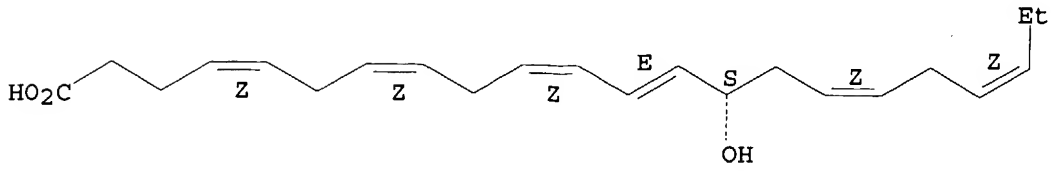
RN 92693-03-3 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, [S-(E,Z,Z,Z,Z,Z)]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



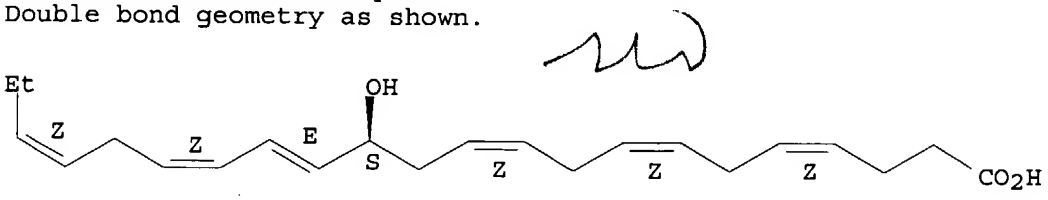
RN 119433-37-3 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,14S,16Z,19Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



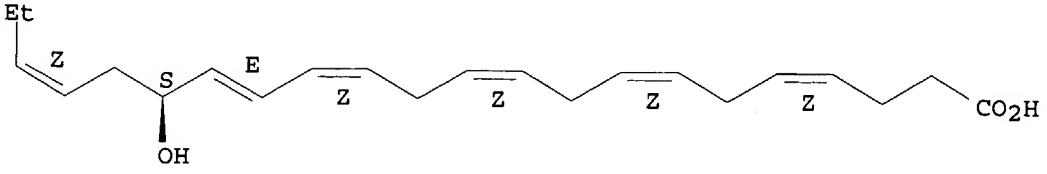
RN 139974-01-9 HCAPLUS
CN 4,7,10,14,16,19-Docosahexaenoic acid, 13-hydroxy-, [S-(E,Z,Z,Z,Z,Z)]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L28 ANSWER 29 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1991:534869 HCAPLUS
DOCUMENT NUMBER: 115:134869
TITLE: Inhibitory potencies of fish oil hydroxy fatty acids on cellular lipoxygenases and platelet aggregation
AUTHOR(S): Vanderhoek, Jacy Y.; Schoene, Norberta W.; Pham, Phi-Phung T.
CORPORATE SOURCE: Sch. Med. Health Sci., George Washington Univ., Washington, DC, USA
SOURCE: Biochemical Pharmacology (1991), 42(4), 959-62
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The presence of dietary eicosapentaenoic acid and/or docosahexaenoic acid can lead to the formation of certain hydroxylated metabolites which are capable of (1) regulating both blood platelet and polymorphonuclear lipoxygenases, and (2) inhibiting platelet aggregation.
IT **92693-03-3 119433-37-3**
RL: BIOL (Biological study)
(of fish oil, cellular lipoxygenases and blood platelet aggregation response to dietary)
RN 92693-03-3 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, [S-(E,Z,Z,Z,Z,Z)]-(9CI) (CA INDEX NAME)

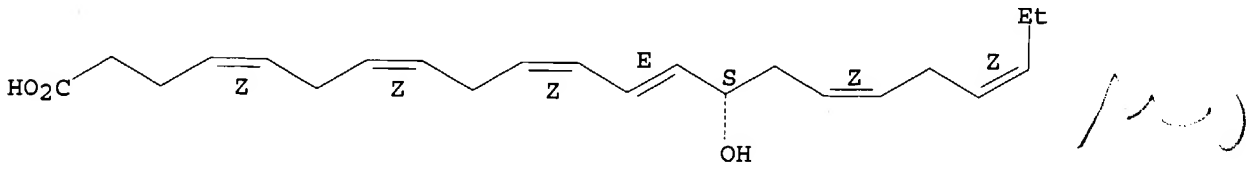
Absolute stereochemistry.
Double bond geometry as shown.



RN 119433-37-3 HCAPLUS

CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,14S,16Z,19Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

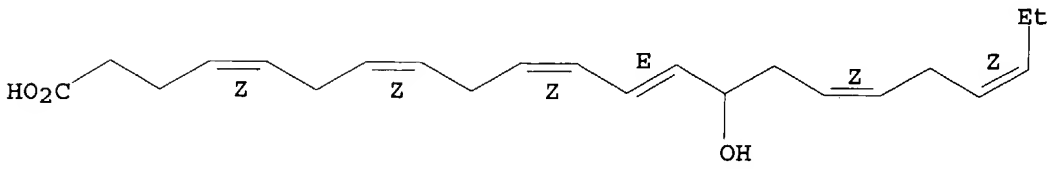


L28 ANSWER 30 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1991:489837 HCAPLUS
DOCUMENT NUMBER: 115:89837
TITLE: Oxidant stress inhibits the endogenous production of lipoxygenase metabolites in rat lungs and fish gills
AUTHOR(S): German, J. Bruce; Hu, Miao Lin
CORPORATE SOURCE: Dep. Food Sci. Technol., Univ. California, Davis, CA, 95616, USA
SOURCE: Free Radical Biology & Medicine (1990), 8(5), 441-8
CODEN: FRBMEH; ISSN: 0891-5849
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Hydroperoxides are potent initiators of lipid peroxidn. in vivo. Acyl hydroperoxides may also regulate various aspects of lipid metabolism The regulation of the endogenous 12 lipoxygenase in trout gill and rat lung, a prominent acyl hydroperoxide catalyst in these tissues, was investigated. Initial expts. revealed that the enzyme from trout gill was activated by hydroperoxides at low levels and inactivated by the same hydroperoxides at high levels. Homogenization of these tissues resulted in the production of a predominant metabolite class from released endogenous polyunsatd. fatty acids, the 12 lipoxygenase products. In rat lung, arachidonic acid was the major polyunsatd. fatty acid released and 12(S)-HETE was the major metabolite. In trout gill 20:4, 20:5 (n3), and 22:6 (n3) were released and the 12(S), 12, and 14 hydroxy derivs. were the corresponding metabolites. Computer simulations of the sensitivity of these enzymes to hydroperoxides predicted that exogenous oxidant stress would reduce significantly the production of HETEs. tert-Bu hydroperoxide was added to tissue homogenates and resulted in elimination of >95% of the lipoxygenase activity. Apparently, the lipoxygenase enzyme in lung and gill tissue is a major potential source for acyl hydroperoxides in vivo, but is also very sensitive to oxidant stresses including the acyl hydroperoxides themselves. This enzyme could thus be an important focus for oxidant injury in lungs.

IT **87042-40-8**
RL: FORM (Formation, nonpreparative)
(formation of, by lipoxygenase of gill of fish and lung of mammal, hydroperoxide effect on)
RN 87042-40-8 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



29

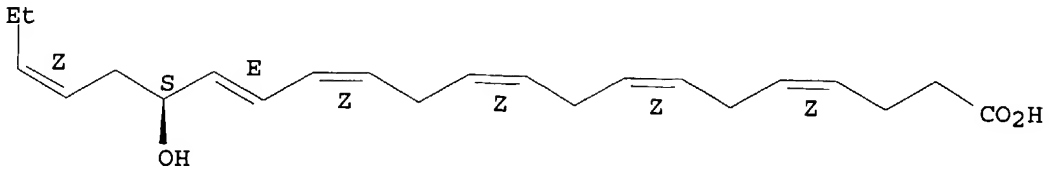
L28 ANSWER 31 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1991:205907 HCAPLUS
DOCUMENT NUMBER: 114:205907
TITLE: Dietary supplementation with ethyl ester concentrates of fish oil (n-3) and borage oil (n-6) polyunsaturated fatty acids induces epidermal generation of local putative anti-inflammatory metabolites
AUTHOR(S): Miller, Craig C.; Tang, Wilson; Ziboh, Vincent A.; Fletcher, Mark P.
CORPORATE SOURCE: Davis Sch. Med., Univ. California, Davis, CA, 95616, USA
SOURCE: Journal of Investigative Dermatology (1991), 96(1), 98-103
CODEN: JIDEAE; ISSN: 0022-202X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Clin. reports have attributed the amelioration of chronic inflammatory skin disorders to the presence of certain polyunsatd. fatty acids (PUFA) in dietary oils. To test the hypothesis of a local modulatory effect of these PUFA in the epidermis, the basal diet of normal guinea pigs was supplemented with Et esters of either fish oil [rich in eicosapentaenoic acid (EPA) and docosahexaenoic acid (DHA)] or borage oil [rich in gamma-linolenic acid (GLA)]. The data demonstrated that dietary oils influence the distribution of PUFA in epidermal phospholipids and the epidermal levels of PUFA-derived hydroxy fatty acids. Specifically, animals supplemented with Et esters of fish oil markedly incorporated EPA and DHA into epidermal phospholipids, which paralleled the epidermal accumulation of 15-hydroxyeicosapentaenoic acid (15-HEPE) and 17-hydroxydocosahexaenoic acid (17-HDoHE). Similarly, animals supplemented with esters of borage oil preferentially incorporated dihomogammalinolenic acid (DGLA), and epidermal elongase product of GLA, into the epidermal accumulation of 15-hydroxyeicosatrienoic acid (15-HETrE). By factoring the epidermal levels of the 15-lipoxygenase products and their relative inhibitory potencies, a measure was evolved of the overall potential of dietary oils to exert local anti-inflammatory effect. For example, the leukotriene inhibition potentials (LIP) of both fish oil and borage oil were greatly enhanced when compared to controls. Thus, the altered profiles of epidermal 15-lipoxygenase products generated from particular dietary oils may be responsible, at least in part, for reported ameliorative effects of oils on chronic inflammatory skin disorders.

IT **92693-03-3**
RL: FORM (Formation, nonpreparative)
(formation of, in skin epidermis during inflammation, dietary Et ester concs. of fish oil and borage oil polyunsatd. fatty acids effect on)
RN 92693-03-3 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, [S-(E,Z,Z,Z,Z,Z)]-(9CI) (CA INDEX NAME)

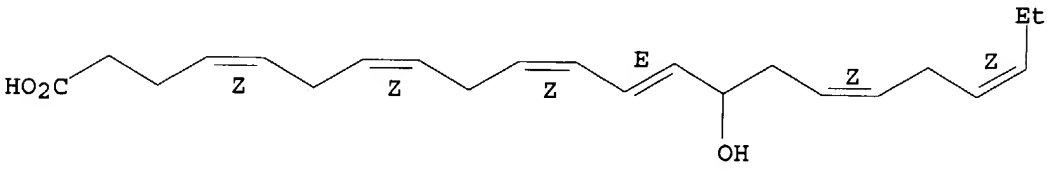
Absolute stereochemistry.

Double bond geometry as shown.



L28 ANSWER 32 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1991:182412 HCAPLUS
DOCUMENT NUMBER: 114:182412
TITLE: Hydroxyeicosatetraenoic, hydroxyeicosapentaenoic, hydroxydocosapentaenoic, and hydroxydocosahexaenoic acids from the sponge Echinochalina mollis of the Coral Sea [Erratum to document cited in CA113(7):56032f]
AUTHOR(S): Guerriero, Antonio; D'Ambrosio, Michele; Pietra, Francesco; Ribes, Olivier; Duhet, Daniel
CORPORATE SOURCE: Ist. Chim., Univ. Trento, Povo-Trento, 38050, Italy
SOURCE: Journal of Natural Products (1990), 53(5), 1181
CODEN: JNPRDF; ISSN: 0163-3864
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Errors in the stereochem. of compds. 1, 3, and 4 have been corrected The errors were reflected in the abstract and index entries.
IT **87042-40-8**
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of sponge (Erratum))
RN 87042-40-8 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

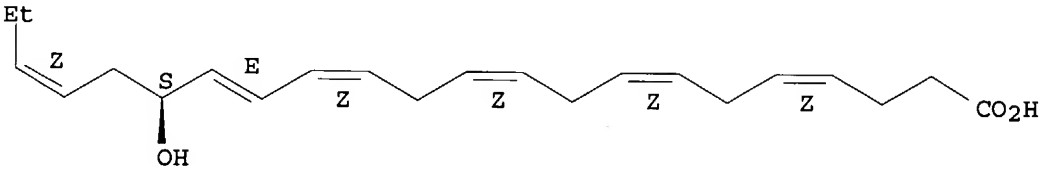


L28 ANSWER 33 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1991:59520 HCAPLUS
DOCUMENT NUMBER: 114:59520
TITLE: Formation of 15-lipoxygenase product from docosahexaenoic acid (22:6w3) by human platelets
AUTHOR(S): Kim, H. Y.; Karanian, J. W.; Salem, N., Jr.
CORPORATE SOURCE: Sect. Anal. Chem., NIAAA, Bethesda, MD, 20892, USA
SOURCE: Prostaglandins (1990), 40(5), 539-49
CODEN: PRGLBA; ISSN: 0090-6980
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The metabolism of docosahexaenoic acid (22:6w3) by 15-lipoxygenase activity of washed human platelets was investigated. Platelets produced

17-hydroxydocosahexaenoic acid when incubated with 22:6w3. Similarly, 15-hydroxyeicosatetraenoic acid and 13- and 9-hydroxyoctadecadienoic acids (HODD) were produced when incubated with 20:4w6 and 18:2w6, resp. However, these products were observed only as minor components in the platelet incubation mixture Control studies with carefully purified platelets and mononuclear cells indicated that these products were formed by the platelets. Chiral phase HPLC anal. indicated that these compds. were mainly in the S configuration with the exception of the 9-HODD, thus, confirming that a lipoxygenase is responsible for their production The 9-HODD produced by platelets was a racemic mixture

IT **92693-03-3**
RL: FORM (Formation, nonpreparative)
(formation of, from docosahexaenoic acid by blood platelet of human)
RN 92693-03-3 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, [S-(E,Z,Z,Z,Z,Z)]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

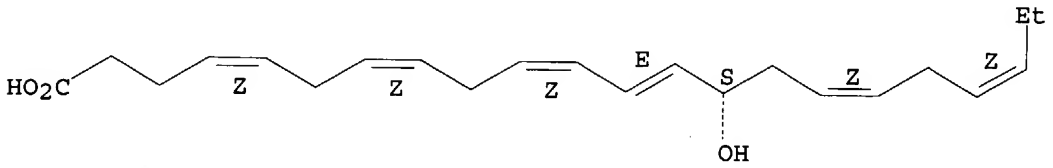


L28 ANSWER 34 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1991:39806 HCAPLUS
DOCUMENT NUMBER: 114:39806
TITLE: Stereochemical analysis of hydroxylated docosahexaenoates produced by human platelets and rat brain homogenate
AUTHOR(S): Kim, H. Y.; Karanian, J. W.; Shingu, T.; Salem, N., Jr.
CORPORATE SOURCE: Sect. Anal. Chem., NIAAA, Bethesda, MD, 20892, USA
SOURCE: Prostaglandins (1990), 40(5), 473-90
CODEN: PRGLBA; ISSN: 0090-6980
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The stereochem. configuration of hydroxylated products of docosahexaenoic acid (22:6ω3) formed by human platelets and rat brain homogenate were characterized for the first time. Chiral phase HPLC was employed along with autoxidized 22:6ω3 as reference material. The 14- and 11-hydroy 22:6ω3 (HDHE) products produced by human platelets were in the S configuration. Rat brain homogenate produced all of the 10 possible positional isomers when incubated with 22:6ω3. Their retention behavior on the reversed and chiral phase HPLC columns and GC/MS/EI anal. indicated that they were 20-, 17-, 16-, 14-, 13-, 11-, 10-, 8-, 7- and 4-HDHE. However, stereochem. anal. revealed that each positional isomer was a racemic mixture, suggesting that these were not formed by lipoxygenation but mainly by peroxidn. process.

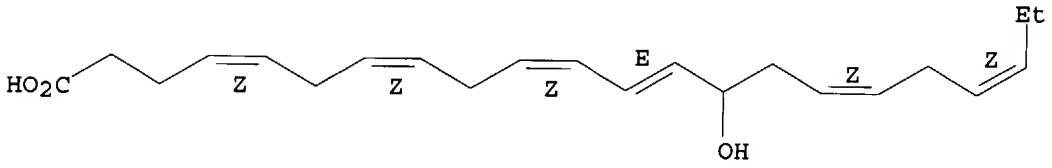
IT **119433-37-3**
RL: FORM (Formation, nonpreparative)
(formation of, by blood platelet of human)
RN 119433-37-3 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,14S,16Z,19Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



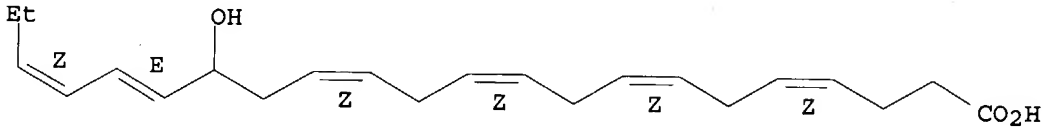
IT **87042-40-8 90780-51-1 90780-52-2**
90780-53-3 90906-41-5
RL: FORM (Formation, nonpreparative)
(formation of, by brain)
RN 87042-40-8 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



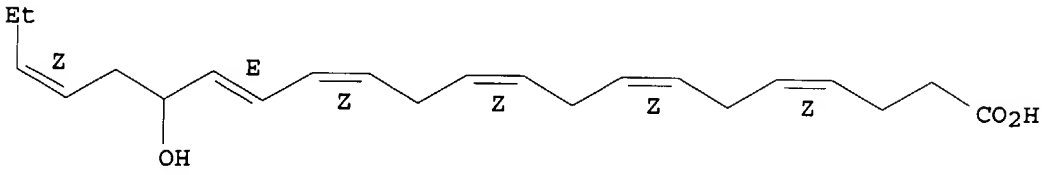
RN 90780-51-1 HCAPLUS
CN 4,7,10,13,17,19-Docosahexaenoic acid, 16-hydroxy-, (4Z,7Z,10Z,13Z,17E,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



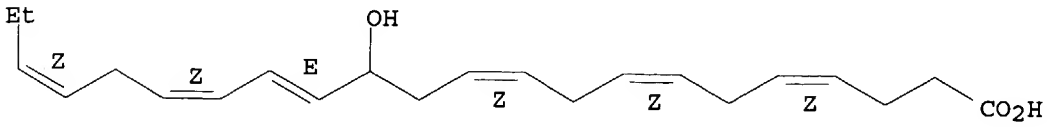
RN 90780-52-2 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, (4Z,7Z,10Z,13Z,15E,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 90780-53-3 HCAPLUS
CN 4,7,10,14,16,19-Docosahexaenoic acid, 13-hydroxy-, (4Z,7Z,10Z,14E,16Z,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.

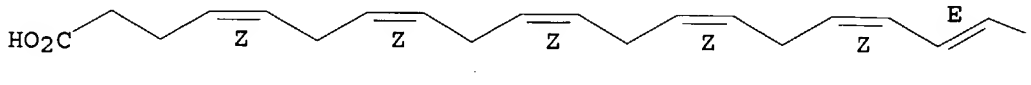


28

RN 90906-41-5 HCAPLUS
CN 4,7,10,13,16,18-Docosahexaenoic acid, 20-hydroxy-, (4Z,7Z,10Z,13Z,16Z,18E)-(9CI) (CA INDEX NAME)

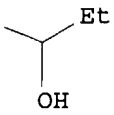
Double bond geometry as shown.

PAGE 1-A



32

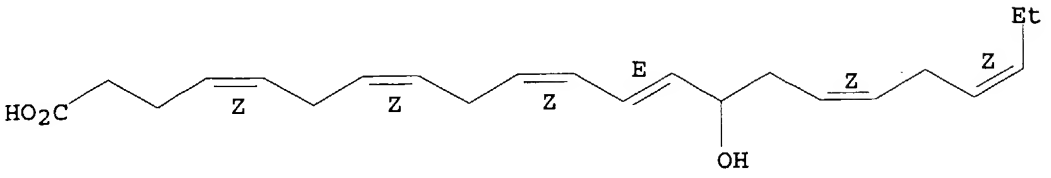
PAGE 1-B



L28 ANSWER 35 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1990:456032 HCAPLUS
DOCUMENT NUMBER: 113:56032
TITLE: Hydroxyeicosatetraenoic, hydroxyeicosapentaenoic, hydroxydocosapentaenoic, and hydroxydocosahexaenoic acids from the sponge Echinochalina mollis of the Coral Sea
AUTHOR(S): Guerriero, Antonio; D'Ambrosio, Michele; Pietra, Francesco; Ribes, Olivier; Duhet, Daniel
CORPORATE SOURCE: Ist. Chim., Univ. Trento, Povo-Trento, 38050, Italy
SOURCE: Journal of Natural Products (1990), 53(1), 57-61
CODEN: JNPRDF; ISSN: 0163-3864
DOCUMENT TYPE: Journal
LANGUAGE: English
AB It is reported that the demosponge E. millis contains in relatively large amts. (+)-(12R,5Z,8Z,10E,14Z,17Z)-12-hydroxy-5,8,10,14,17-eicosapentaenoic acid, (+)-(12S,5Z,8Z,10E,14Z)-12-hydroxy-5,8,10,14-eicosatetraenoic acid, (+)-(12R,4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxy-4,7,10,12,16,19-docosahexaenoic acid, and (+)-(12R,4Z,7Z,10Z,12E,16Z)-14-hydroxy-4,7,10,12,16-docosapentaenoic acid. The latter three acids are detected for the first time in a marine invertebrate.
IT **87042-40-8**
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of sponge)
RN 87042-40-8 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)-(9CI) (CA INDEX NAME)

29

Double bond geometry as shown.



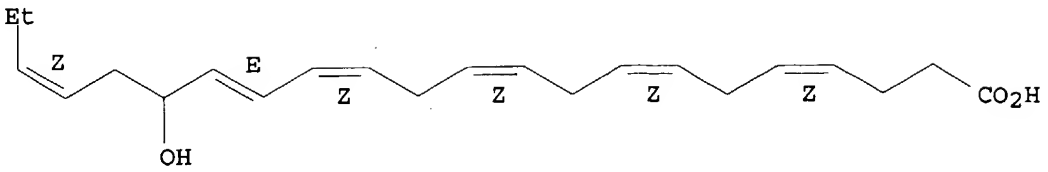
L28 ANSWER 36 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1990:117061 HCAPLUS
DOCUMENT NUMBER: 112:117061
TITLE: Guinea pig epidermis generates putative anti-inflammatory metabolites from fish oil polyunsaturated fatty acids
AUTHOR(S): Miller, Craig C.; Yamaguchi, Ronald Y.; Ziboh, Vicent A.
CORPORATE SOURCE: Sch. Med., Univ. California, Davis, CA, 95616, USA
SOURCE: Lipids (1989), 24(12), 998-1003
CODEN: LPDSAP; ISSN: 0024-4201
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Clin. studies have indicated that dietary fish oil may have therapeutic value in the treatment of psoriasis, a hyperproliferative, inflammatory skin disorder characterized by elevated LTB4. To evolve a possible mechanism for these beneficial effects, the metabolic fate of fish oil-derived n-3 fatty acids was determined in the skin. Specifically, guinea pig epidermal enzyme prepns. were incubated with [3H]eicosapentaenoic acid (20:5n-3) and [14C]docosahexaenoic acid (22:6n-3). Analyses of the radiometabolites revealed the transformation of these n-3 fatty acids into n-6 lipoxygenase (arachidonate 15-lipoxygenase) products: 15-hydroxyeicosapentaenoic acid (15-HEPE) and 17-hydroxydocosahexaenoic acid (17-HDHE), resp. Since 15-lipoxygenase products have been suggested to be possible endogenous inhibitors of 5-lipoxygenase (an enzyme which catalyzes the formation of LTB4), the ability of 15-HEPE and 17-HDHE in vitro to inhibit the activity of the 5-lipoxygenase was tested. Incubations of these metabolites with enzyme prepns. from rat basophilic leukemia (RBL-1) cells demonstrated that 15-HEPE (50% inhibitory concentration (IC50) = 28 μM) and 17-HDHE (IC50 = 25 μM) are potent inhibitors of the RBL-1 5-lipoxygenase. The inhibitory potential of these fish oil metabolites provides a possible mechanism by which fish oil might act to decrease local cutaneous levels of LTB4, and thereby alleviate psoriatic symptoms.

IT **90780-52-2**
RL: FORM (Formation, nonpreparative)
(formation of, from polyunsatd. fatty acids of fish oil in skin epidermis, LTB4 formation inhibition and psoriasis therapy in relation to)
RN 90780-52-2 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, (4Z,7Z,10Z,13Z,15E,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.

30

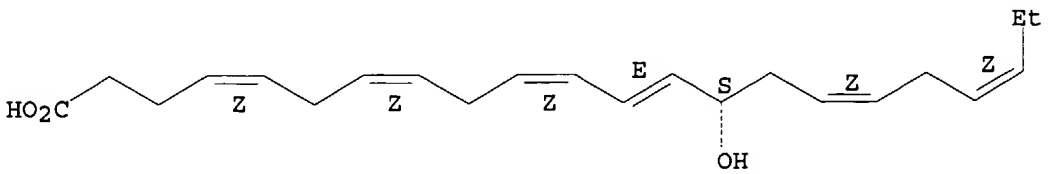


L28 ANSWER 37 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1989:608865 HCAPLUS
DOCUMENT NUMBER: 111:208865
TITLE: Cardiovascular properties of hydroxylated docosahexaenoates
AUTHOR(S): Karanian, John W.; Kim, Hee Yong; Shingu, Tadashi; Yergey, James; Salem, Norman, Jr.
CORPORATE SOURCE: Lab. Clin. Stud., Natl. Inst. Alcohol Abuse Alcohol., Bethesda, MD, 20892, USA
SOURCE: Progress in Clinical and Biological Research (1989), 301(Prostaglandins Clin. Res.: Cardiovasc. Syst.), 511-15
CODEN: PCBRD2; ISSN: 0361-7742
DOCUMENT TYPE: Journal
LANGUAGE: English

AB In rat and rabbit aorta, contraction induced by the thromboxane agonist U46619 was inhibited by pretreatment with hydroxylated docosahexaenoates (14-hydroxy derivative > 17 hydroxy derivative > 11-hydroxy derivative). In comparison, 12-HETE was inhibitory only at a concentration an order of magnitude higher. The pharmacol. action of the hydroxylated docosahexaenoates appears to depend upon the position of the hydroxy group, indicating a relatively specific antithromboxane activity. These results indicate that 12-lipoxygenase metabolites of docosahexaenoate may have physiol. importance. The enzymic preparation of hydroxydocosahexaenoic acids by using soybean lipoxygenase and blood platelets is described.

IT **119433-37-3**
RL: FORM (Formation, nonpreparative)
(formation of, by platelets of humans and laboratory animals and as vasodilator, structure in relation to)
RN 119433-37-3 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,14S,16Z,19Z)- (9CI) (CA INDEX NAME)

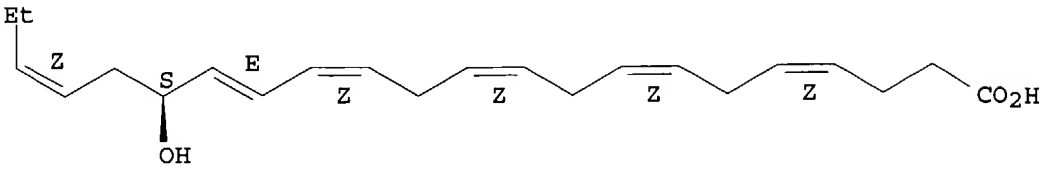
Absolute stereochemistry.
Double bond geometry as shown.



IT **92693-03-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of and as vasodilator, structure in relation to)
RN 92693-03-3 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, [S-(E,Z,Z,Z,Z,Z)]-

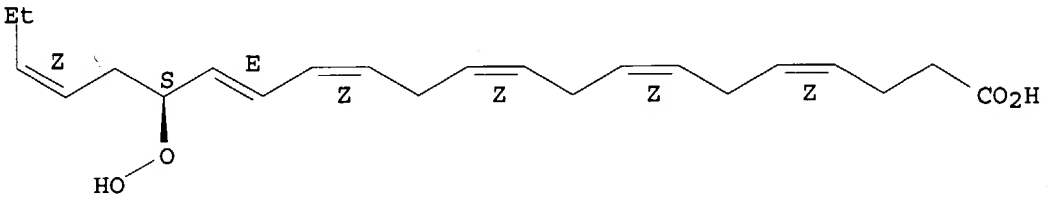
(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



IT **123673-33-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of)
RN 123673-33-6 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroperoxy-,
(4Z,7Z,10Z,13Z,15E,17S,19Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

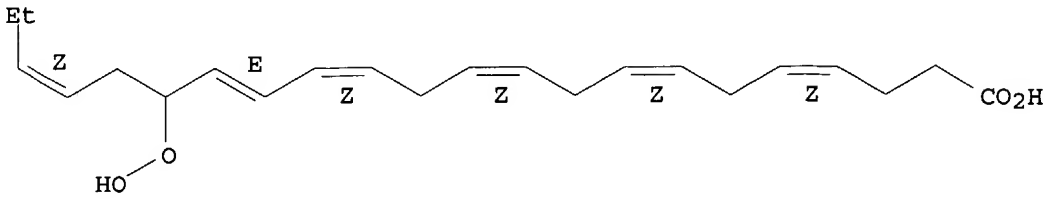


L28 ANSWER 38 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1989:450483 HCAPLUS
DOCUMENT NUMBER: 111:50483
TITLE: Preparation and the structural determination of hydroperoxy derivatives of docosahexaenoic acid and other polyunsaturates by thermospray LC/MS
AUTHOR(S): Kim, H. Y.; Salem, N., Jr.
CORPORATE SOURCE: DICBR, NIAAA, Bethesda, MD, 20892, USA
SOURCE: Prostaglandins (1989), 37(1), 105-19
CODEN: PRGLBA; ISSN: 0090-6980
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A new method to determine the structure of lipoxygenase reaction products is presented. Thermospray mass spectra (MS) of hydroperoxy derivs. of polyunsaturates contain both mol. ion species and fragments reflecting the position of oxygenation. Data are presented for hydroperoxy-docosahexaenoic, eicosapentaenoic, arachidonic and linoleic acids in this regard. Ten positional isomers of hydroperoxydocosahexaenoic acid were prepared by autoxidn. and their structures were determined by thermospray HPLC/MS
and confirmed by electron impact gas chromatog./MS after suitable derivs. were made. This technique was particularly useful in determining the structure of unknown metabolites by direct monitoring of the reaction mixture without derivatization. The value of this approach was demonstrated using a soybean lipoxygenase reaction mixture as a simple example.
IT **70596-95-1 121694-99-3 121695-00-9**
121695-01-0 121695-02-1

RL: ANT (Analyte); ANST (Analytical study)
(structure determination of, by thermospray mass spectra, from lipoxygenase reaction products)

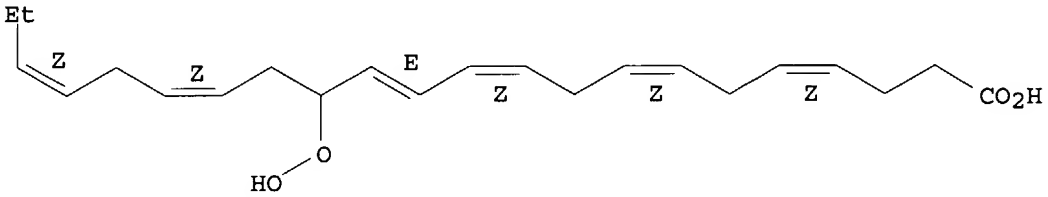
RN 70596-95-1 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroperoxy-, (4Z,7Z,10Z,13Z,15E,19Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



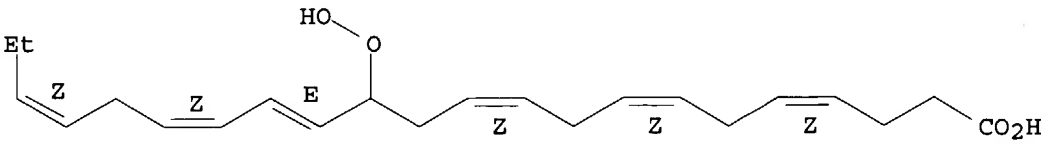
RN 121694-99-3 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroperoxy-, (E,Z,Z,Z,Z,Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



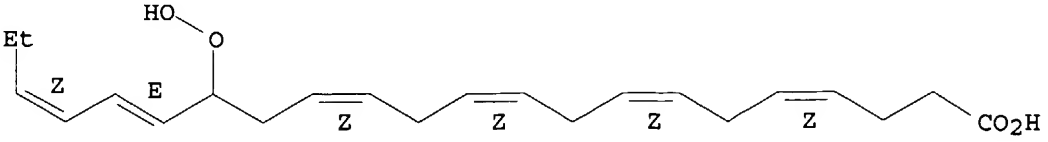
RN 121695-00-9 HCAPLUS
CN 4,7,10,14,16,19-Docosahexaenoic acid, 13-hydroperoxy-, (E,Z,Z,Z,Z,Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 121695-01-0 HCAPLUS
CN 4,7,10,13,17,19-Docosahexaenoic acid, 16-hydroperoxy-, (E,Z,Z,Z,Z,Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

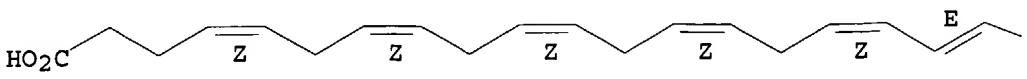


RN 121695-02-1 HCAPLUS

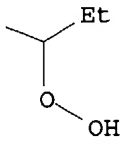
CN 4,7,10,13,16,18-Docosahexaenoic acid, 20-hydroperoxy-, (E,Z,Z,Z,Z,Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



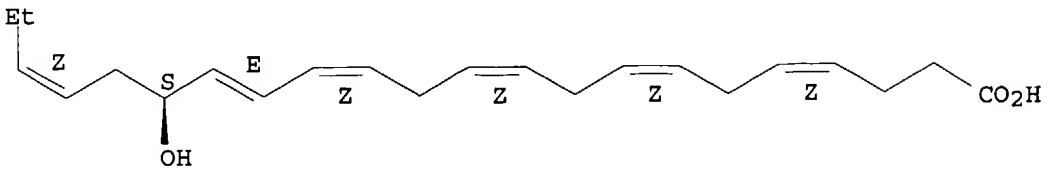
L28 ANSWER 39 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1989:421226 HCAPLUS
DOCUMENT NUMBER: 111:21226
TITLE: Metabolism of polyunsaturated fatty acids by an (n-6)-lipoxygenase associated with human ejaculates
AUTHOR(S): Oliw, Ernst H.; Sprecher, Howard
CORPORATE SOURCE: Dep. Pharmacol., Karolinska Inst., Stockholm, S-104 01, Swed.
SOURCE: Biochimica et Biophysica Acta (1989), 1002(3), 283-91
CODEN: BBACAQ; ISSN: 0006-3002
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Washed cells of normal human ejaculates were incubated with [14C]arachidonic acid (20:4(n-6)) at 37° for 30-40 min and the main product was characterized as 15(S)-hydroxy-5,8,11,13-eicosatetraenoic acid by reverse-phase, straight-phase and chiral-phase HPLC and by capillary gas chromatog.-mass spectrometry. The biosynthesis of 15(S)-hydroxy-5,8,11,13-eicosatetraenoic acid from exogenous 20:4(n-6) was inhibited by nordihydroguaiaretic acid and abolished by heat inactivation, but it appeared to be unaffected by the ionophore A 23187 and Ca2+. Human spermatozoa were partly purified from contaminating material by the swim-up procedure and incubated with 14C-labeled 18:2(n-6), 20:4(n-6), 22:5(n-6), and 22:6(n-3) for 30-40 min at 37°. The main radiolabeled products, which were obtained in low yields, cochromatographed with the Ls(n-6)-hydroxy fatty acid of each substrate on reverse-phase, straight-phase and chirla-phase HPLC. The (n-6)-lipoxygenase was also present in ejaculates with oligozoospermia or azoospermia. The seminal fluid contains membrane-surrounded organelles (e.g., prostasomes secreted by the prostate gland) and the (n-6)-lipoxygenase was present and appeared to be relatively prominent in almost cell-free prepns. of organelles of seminal fluid. The (n-6)-lipoxygenase activity associated with the spermatozoa may thus be explained by the presence of prostasomes or other organelles, which may conceivably bind to the spermatozoon through hydrophobic interactions.

IT **92693-03-3**
RL: FORM (Formation, nonpreparative)
(formation of, from polyunsatd. fatty acid by (n-6)-lipoxygenase associated with human semen)

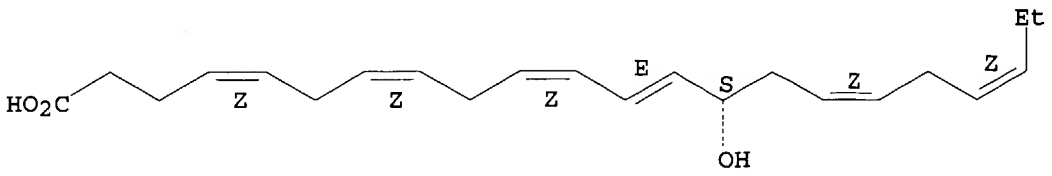
RN 92693-03-3 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, [S-(E,Z,Z,Z,Z,Z)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L28 ANSWER 40 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1989:108908 HCAPLUS
DOCUMENT NUMBER: 110:108908
TITLE: Smooth muscle effects of hydroxylated docosahexaenoates produced from human platelet
AUTHOR(S): Karanian, J. W.; Kim, H. Y.; Shingu, T.; Yergey, J. A.; Yoffe, A.; Salem, N., Jr.
CORPORATE SOURCE: Lab. Clin. Stud., Natl. Inst. Alcohol Abuse and Alcoholism, Bethesda, MD, 20892, USA
SOURCE: Biomedica Biochimica Acta (1989), 47(10-11), S79-S82
CODEN: BBIADT; ISSN: 0232-766X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Washed platelets (108 cells/mL) are capable of metabolizing docosahexaenoic acid (22:6w3, DHE) to 12-lipoxygenase derivs. The 2 major metabolites of the DHE thus formed were collected and derivatized for anal. by GC/mass spectroscopy. The structures assigned were 14(S)- and 11(S)-hydroxydocosahexaenoate (HDHE). Addition of 12-lipoxygenase inhibitors such as ETYA inhibited the production of HDHE. The metabolites formed are biol. active as they are capable of inducing a weak contraction in airway but not vascular smooth muscle prepns.; a thromboxane agonist (U46619) was 10-20-fold more efficacious than HDHE in the guinea pig lung parenchymal strip. HDHE may act in part through stimulation of leukotriene production as increased peptidyl-leukotriene levels were associated with the HDHE-induced contraction in this preparation and a lipoxygenase inhibitor (NDGA) was capable of a partial blockade of this response. In addition, HDHE antagonizes the contractile effects of the thromboxane agonist, U46619, especially in vascular smooth muscle. Stimulation of the sulfido-peptido leukotrienes and thromboxane antagonism may therefore be important aspects of the biol. function of HDHE.
IT **119433-37-3**
RL: BIOL (Biological study)
(as docosahexaenoate metabolite, in blood platelets of humans, smooth muscle contraction in relation to)
RN 119433-37-3 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,14S,16Z,19Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

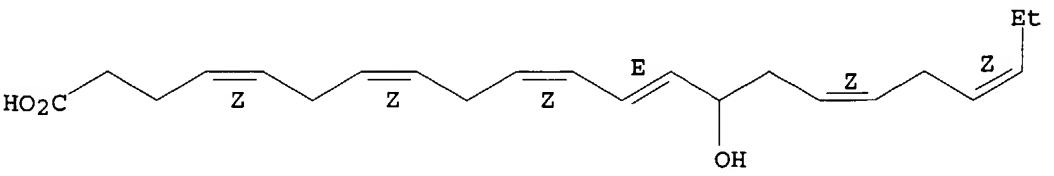


L28 ANSWER 41 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1989:72951 HCAPLUS
DOCUMENT NUMBER: 110:72951
TITLE: Specialization in membrane structure and metabolism with respect to polyunsaturated lipids
AUTHOR(S): Salem, Norman, Jr.; Shingu, Tadashi; Kim, Hee Yong; Hullin, Francoise; Bougnoux, Philippe; Karanian, John W.
CORPORATE SOURCE: Lab. Clin. Stud., Natl. Inst. Alcohol Abuse Alcoholism, Bethesda, MD, 20892, USA
SOURCE: Progress in Clinical and Biological Research (1988), 282(Biol. Membr.: Aberrations Membr. Struct. Funct.), 319-33
CODEN: PCBRD2; ISSN: 0361-7742
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The specialized functions of the polyunsatd. fatty acids C22:6 (n-3) and C20:4 (n-6) is determining cell membrane phys. properties as components of phospholipids and as precursors of oxygenated metabolites enzymically formed from the free acids were examined Polyunsatd. aminophospholipids were nonrandomly distributed in plasma membranes. Human blood platelets incubated with 14C22:6 (n-3) formed 14-hydroxy-C22:6 (n-3) as the major product and 11-hydroxy-C22:6 (n-3) in smaller amts. Rat brain homogenate produced the above products from 14C22:6 (n-3) and addnl. products as well, indicating 5-lipoxygenase activity. Polyunsatd. phospholipids are preferentially localized on the cytosolic leaflet of the cell membrane and around proteins. Released polyunsatd. fatty acids can be metabolized by a lipoxygenase enzyme in blood platelets and brain and the products formed are biol. active.

IT **87042-40-8**
RL: FORM (Formation, nonpreparative)
(formation of, by blood platelets of human and brain of laboratory animals)
RN 87042-40-8 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



L28 ANSWER 42 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1989:69479 HCAPLUS
DOCUMENT NUMBER: 110:69479

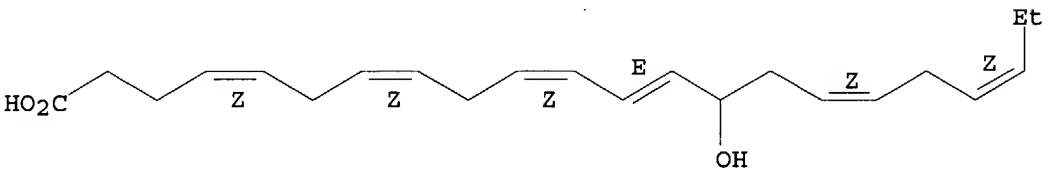
TITLE: Liquid chromatography and gas chromatography/mass spectrometry of lipoxygenase and cycloxygenase products from platelets and endothelial cells
AUTHOR(S): Guichardant, M.; Bordet, J. C.; Lagarde, M.
CORPORATE SOURCE: Inst. Pasteur, Lyon, Fr.
SOURCE: Biomedical & Environmental Mass Spectrometry (1988), Volume Date 1987, 16(1-12), 245-8
CODEN: BEMSEN; ISSN: 0887-6134
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Liquid chromatog. coupled with mass spectrometry using either pos. or neg. ionization was used for measuring various lipoxygenase products of polyunsatd. fatty acids. The neg. ionization appeared as the most sensitive mode and allowed to detect pmol amts. of products from biol. exts. Gas chromatog./mass spectrometry with the neg. chemical ionization mode was also used for measuring prostacyclin synthetase products, namely the stable metabolites of PGI2, PGI3, and dihomo PGI2. In this way, fmol amts. of metabolites could be measured in biol. exts.

IT **87042-40-8**
RL: ANT (Analyte); ANST (Analytical study)
(determination of, in platelets by liquid chromatog.-mass spectroscopy)

RN 87042-40-8 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



L28 ANSWER 43 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1988:434689 HCAPLUS
DOCUMENT NUMBER: 109:34689
TITLE: Thermospray-mass spectrometric analysis of underivatized monohydroxy fatty acids: application to stimulated platelets
AUTHOR(S): Guichardant, Michel; Lagarde, Michel; Lesieur, Michel; De Maack, Frederic
CORPORATE SOURCE: Inst. Pasteur, Fac. Alexis Carrel, Lyon, 69372, Fr.
SOURCE: Journal of Chromatography (1988), 425(1), 25-34
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Monohydroxylated fatty acids prepared from polyunsatd. fatty acids of nutritional value were analyzed by thermospray-mass spectrometry without prior chemical derivatization. Pos. and neg. ionization modes were compared. The highest sensitivity was observed with the neg. ionization mode with detection limits of 10 pmol based on the 12-hydroxy derivs. of eicosatrienoic acid (12-OH-8,10,14-20:3). This is comparable to that obtained by HPLC with UV detection at 234 nm. Selected ion monitoring based on the fragment [M - H]- allowed a variety of standard monohydroxy fatty acids to be detected. This approach makes possible the anal. of various derivs. generated by thrombin-stimulated platelets (109 cells) pre-enriched with minor polyunsatd. fatty acids, even when these derivs.

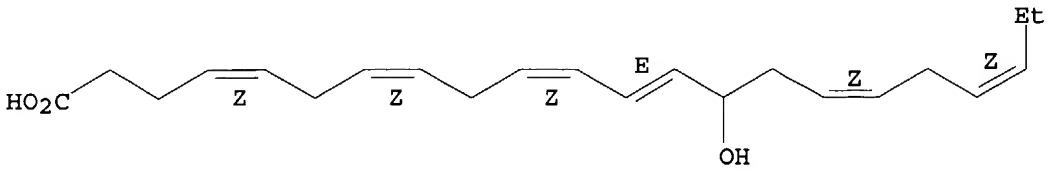
coelute from the column (e.g., 12-HETE and 14-OH-22:6).

IT **87042-40-8**
RL: ANT (Analyte); ANST (Analytical study)
(detection of, in human blood platelets by thermospray-mass spectroscopy)

RN 87042-40-8 HCAPLUS

CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



L28 ANSWER 44 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1988:198935 HCAPLUS

DOCUMENT NUMBER: 108:198935

TITLE: Inhibition by lipoxygenase products of TXA2-like responses of platelets and vascular smooth muscle. 14-Hydroxy from 22:6N-3 is more potent than 12-HETE

AUTHOR(S): Croset, Martine; Sala, Angelo; Folco, Giancarlo; Lagarde, Michel

CORPORATE SOURCE: Fac. Med. Alexis Carrel, Inst. Pasteur, Lyon, Fr.

SOURCE: Biochemical Pharmacology (1988), 37(7), 1275-80
CODEN: BCPCA6; ISSN: 0006-2952

DOCUMENT TYPE: Journal

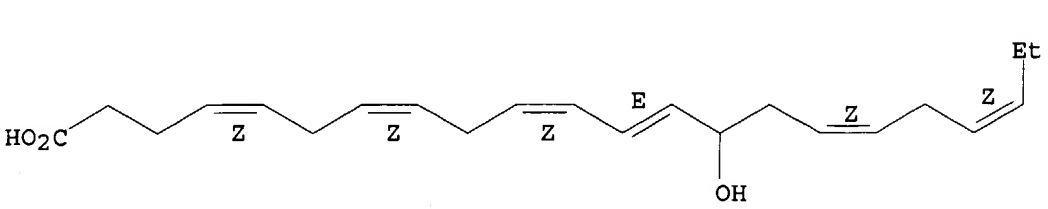
LANGUAGE: English

AB Lipoxygenase products, which are formed in large amts. in platelets during their activation, were prepared from arachidonic acid (20:4n-6), the main polyunsatd. fatty acid (PUFA) esterified in platelet phospholipids, and from 2 major PUFAs of fish fat, eicosapentaenoic (20:5n-3) and docosahexaenoic (22:6n-3) acids. These compds. were synthesized by using platelet suspensions as enzymic source, purified by HPLC, and their structures were checked by gas chromatog.-mass spectrometry. Their effects were investigated in vitro on human platelet aggregation induced by the 11,9-epoxy-methano-analog of PGH2 (U 46619) and on thromboxane A2-induced vasoconstriction of rabbit aorta. All hydroxylated fatty acids inhibited U 46619-induced aggregation in a concentration-dependent fashion. Compds. issued from 22:6n-3 were the most inhibitory and their 50% inhibitory concns. (IC50) differed significantly from that of 12-HETE. Among them, 14-hydroxydocosahexaenoic acid (14-OH-22:6) was the most effective antiaggregating mol. (IC50: 0.45 μM). 12-HETE and 14-OH-22:6 at 10 μM inhibited 60% and 75% of smooth muscle contraction induced by TXA2-like material, resp. At 1 μM, only 14-OH-22:6 had an inhibitory effect on adrenaline-, angiotensin-, and histamine-induced contraction. Since thromboxane receptors in platelets and vascular smooth muscle cells present strong similarities, it is concluded that hydroxylated fatty acids can antagonize prostanoid action probably by interfering with their receptor sites.

IT **87042-40-8**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(artery contraction and human blood platelet aggregation response to thromboxane inhibition by)

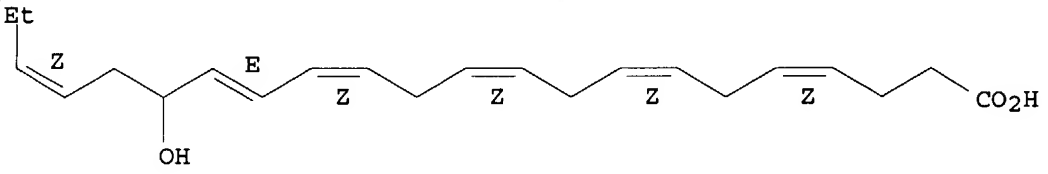
RN 87042-40-8 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)-
(9CI) (CA INDEX NAME)

Double bond geometry as shown.



IT **90780-52-2**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(blood platelet aggregation response to thromboxane inhibition by)
RN 90780-52-2 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, (4Z,7Z,10Z,13Z,15E,19Z)-
(9CI) (CA INDEX NAME)

Double bond geometry as shown.



L28 ANSWER 45 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1988:107032 HCAPLUS
DOCUMENT NUMBER: 108:107032
TITLE: Interference of eicosapentaenoic and docosahexaenoic acids with arachidonate-and U46619-induced platelet activation and desensitization
AUTHOR(S): Hatmi, Mohamed; Lussiana, J. Pierre; Junien, J. Louis; Bure, Jacques; Vargaftig, B. Boris
CORPORATE SOURCE: Inst. Pasteur, INSERM, Paris, 75015, Fr.
SOURCE: Biochemical Pharmacology (1988), 37(3), 481-9
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Eicosapentaenoic acid (EPA) and docosahexaenoic acid (DCHA) suppressed TXB2 formation and prevented activation by arachidonic acid (AA) and U 46619 in human blood platelets. This inhibition required the presence of EPA or DCHA, since platelets pre-treated with these fatty acids and washed before testing responded as controls to the stimulating agents. At 0.1 and 0.3 mM resp., DCHA and EPA behaved as reversible inhibitors of cyclooxygenase or thromboxane synthetase (inhibition of the effects of AA) and as endoperoxides/TXA2 receptor antagonist (inhibition of the effects of U 46619). Coexposure of DCHA (0.1 mM) with AA or U 46619 prevents auto- and cross-desensitization to AA and U 46619. Platelets exposed to 0.3 mM DCHA and washed became refractory to stimulation by AA, but responded as controls to U 46619. EPA (0.3 mM) was fully removed from platelets, which responded to AA and to U 46619. EPA and DCHA antagonize endoperoxide/TXA2 directly, and thus prevent the stimulation-dependent

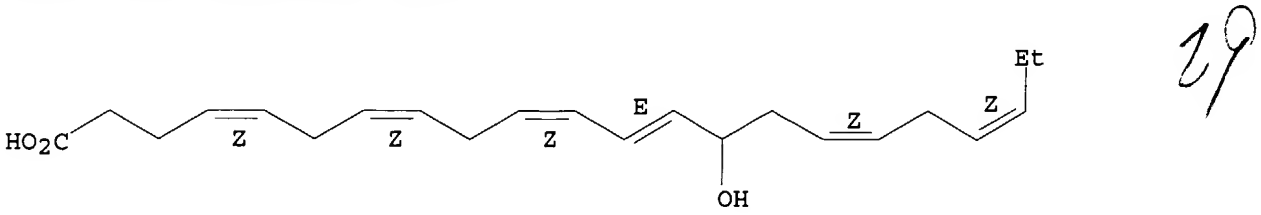
desensitization, and addnl., inhibit the cyclooxygenase activity required for desensitization.

IT **87042-40-8**
RL: BIOL (Biological study)
(as docosahexaenoate metabolite, of blood plasma of human, arachidonate and TXA2-induced activation and desensitization in relation to)

RN 87042-40-8 HCAPLUS

CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



19

L28 ANSWER 46 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1987:452112 HCAPLUS

DOCUMENT NUMBER: 107:52112

TITLE: Diacylglycerols interfere in normal-phase HPLC analysis of lipoxygenase products of docosahexaenoic or arachidonic acids

AUTHOR(S): Claeys, Magda; Bazan, Haydee E. P.; Birkle, Dale L.; Bazan, Nicolas G.

CORPORATE SOURCE: Sch. Med., Louisiana State Univ., New Orleans, LA, 70112, USA

SOURCE: Prostaglandins (1986), 32(6), 813-27
CODEN: PRGLBA; ISSN: 0090-6980

DOCUMENT TYPE: Journal

LANGUAGE: English

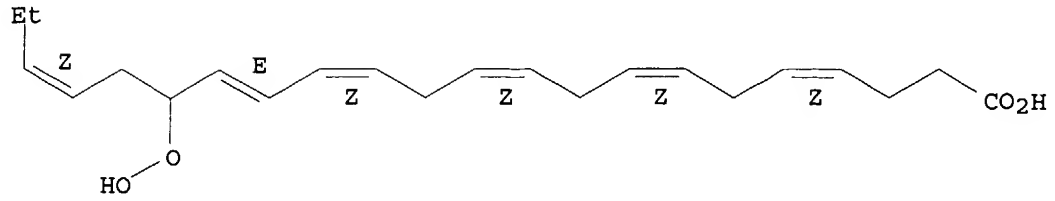
AB A methodol. problem with the normal phase HPLC of hydroxylated products of docosahexaenoic and arachidonic acids is described. Diacylglycerols present in lipid exts. of rat retina co-elute with monohydroxy derivs. of docosahexaenoic or arachidonic acid, when samples are applied to columns and eluted with hexane/iso-POH/AcOH. Anal. of fatty acid composition of diacylglycerols which were Me2CO-extracted from the incubation medium showed a profile similar to diacylglycerols extracted from the tissue by hexane/isopropanol, although Me2CO extraction resulted in extremely variable recovery of diacylglycerols. This co-elution of diacylglycerols with monohydroxy polyunsatd. fatty acids can lead to a significant error in estimation of lipoxygenation activity by conversion of radiolabeled precursors, because the incorporation of fatty acids into diacylglycerols is very active in many tissues. An alternative extraction method and reversed-phase HPLC procedures that result in the complete separation of hydroxy fatty acids and diacylglycerols are described.

IT **70596-95-1 87042-40-8 90780-52-2**
RL: ANT (Analyte); ANST (Analytical study)
(determination of, by normal-phase HPLC, diacylglycerides interference in)

RN 70596-95-1 HCAPLUS

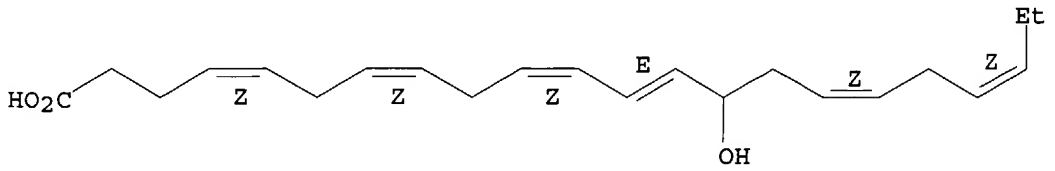
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroperoxy-, (4Z,7Z,10Z,13Z,15E,19Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



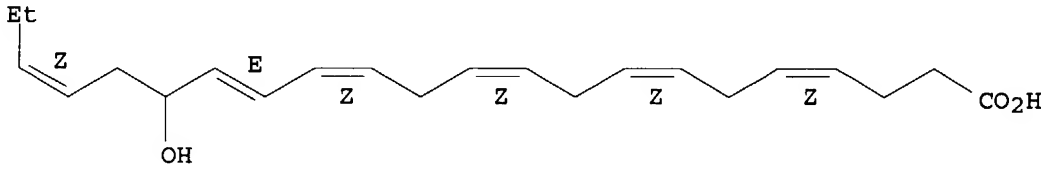
RN 87042-40-8 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 90780-52-2 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, (4Z,7Z,10Z,13Z,15E,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.

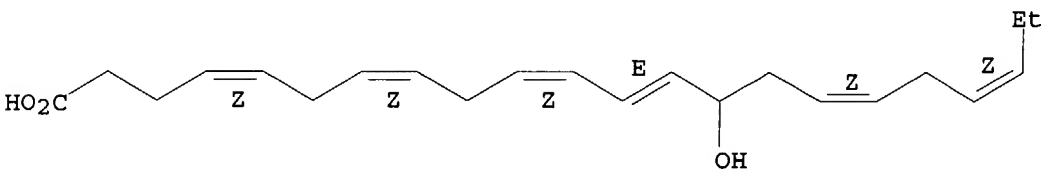


L28 ANSWER 47 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1987:47716 HCAPLUS
DOCUMENT NUMBER: 106:47716
TITLE: Role of lipoxygenase products in platelet function: relation to fatty acid modified phospholipids
AUTHOR(S): Lagarde, Michel; Croset, Martine; Guichardant, Michel; Dechavanne, Marc
CORPORATE SOURCE: Faculte Alexis Carrel, Inst. Pasteur, Lyon, 69372, Fr.
SOURCE: Advances in Experimental Medicine and Biology (1985), 192(Mech. Stimulus-Response Coupling Platelets), 327-35
CODEN: AEMBAP; ISSN: 0065-2598
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Lipoxygenase products of polyunsatd. fatty acids, in particular eicosaenoic acids, can modulate PGH2/TxA2-induced platelet aggregation specifically. Expts. with platelets in vitro enriched with certain eicosaenoic acids rather than arachidonic acid suggest that the corresponding lipoxygenase products could be produced inside the cells at concns. which may induce such modulations. The potentiating concns. of the 12-hydroxy derivative of 20:3 n-9 upon platelet aggregation (<5 +

10-7M) fit well with the quantities of such a derivative produced by 20:3n-9-rich platelets at physiol. concns. during their activation by thrombin or the ionophore, at least at the early stages. In contrast, the 12-hydroxy derivative of 20:5 n-3, which inhibits platelet aggregation at <5 + 10--7M, makes relevant its biosynthesis in 20:5n-3- rich platelets, in terms of platelet inhibition. As the lipoxygenase of 20:3 n-6 is less efficient and its 12-hydroxy derivative is less inhibitory, it is unlikely that the biol. effect of this eicosaenoic acid is due to its lipoxygenase end-product. It could rather be due to its cyclooxygenase metabolites, possibly PGE1.

IT **87042-40-8**
RL: BIOL (Biological study)
(methano-PGH2 derivative-induced blood platelet aggregation inhibition by)
RN 87042-40-8 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



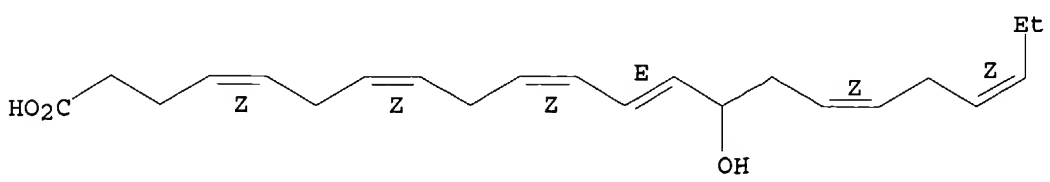
19

L28 ANSWER 48 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1987:47397 HCAPLUS
DOCUMENT NUMBER: 106:47397
TITLE: Bioconversion of docosahexaenoic acid into its 14-hydroxy derivative in rainbow trout gills (Salmo gairdneri, Rich)
AUTHOR(S): Leger, Claude; Linard, Alain; Lagarde, Michel; Guichardant, Michel
CORPORATE SOURCE: Stn. Rech. Nutr., INRA, Jouy-en-Josas, 78350, Fr.
SOURCE: Revue Francaise des Corps Gras (1986), 33(6-7), 269-72
CODEN: RFCGAE; ISSN: 0035-3000
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Fish gill was able to bioconvert 22:6 (n-3) acid into 14-hydroxy-22:6 (n-3) acid, proving that lipoxygenation takes places at position (n-9) of the acyl chain as previously shown in human platelets.

IT **87042-40-8**
RL: FORM (Formation, nonpreparative)
(formation of, from docosahexaenoate by gill of rainbow trout)
RN 87042-40-8 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)-(9CI) (CA INDEX NAME)

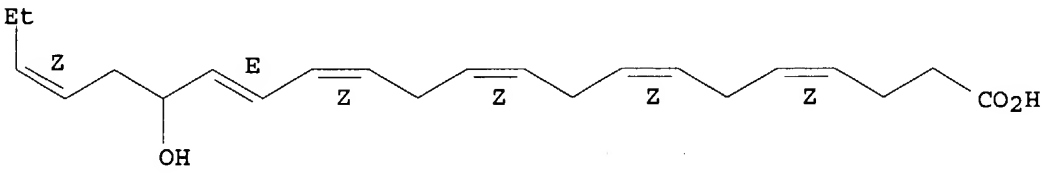
Double bond geometry as shown.



19

L28 ANSWER 49 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1986:589601 HCAPLUS
DOCUMENT NUMBER: 105:189601
TITLE: Lipoxygenase-catalyzed oxidation of N-6 and N-3 polyunsaturated fatty acids: relevance to and activity in fish tissue
AUTHOR(S): Hsieh, R. J.; Kinsella, J. E.
CORPORATE SOURCE: Inst. Food Sci., Cornell Univ., Ithaca, NY, 14853, USA
SOURCE: Journal of Food Science (1986), 51(4), 940-5, 996
CODEN: JFDSAZ; ISSN: 0022-1147
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Lipid peroxidn. is an important process responsible for the flavor deterioration of many plant and animal foods. To understand possible mechanisms of initiation, a soybean lipoxygenase [9029-60-1]-polyunsatd. fatty acid model system was studied. The rate of enzyme-initiated oxidation was monitored by both O consumption and diene conjugation. The hydroperoxides from an n-6 fatty acid, i.e. arachidonic [506-32-1], and n-3 fatty acids, i.e. linolenic [463-40-1], eicosapentaenoic [10417-94-4], and docosahexaenoic acids [6217-54-5] were reduced and analyzed by reverse-phase high pressure liquid chromatog. and gas chromatog./mass spectrometry. The lipoxygenase specifically catalyzed oxygenation at the n-6 C atom of both n-3 and n-6 fatty acids. Lipoxygenase activity was demonstrated in skin homogenate from rainbow trout, and its role in off-flavor development is discussed.
IT **90780-52-2**
RL: FORM (Formation, nonpreparative)
(formation of, in docosahexaenoic acid oxidation by lipoxygenase)
RN 90780-52-2 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, (4Z,7Z,10Z,13Z,15E,19Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L28 ANSWER 50 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1986:565809 HCAPLUS
DOCUMENT NUMBER: 105:165809
TITLE: Metabolism of (n-6) and (n-3) polyunsaturated fatty acids by human platelets
AUTHOR(S): Sprecher, Howard; Careaga, Maria Monica
CORPORATE SOURCE: Dep. Physiol. Chem., Ohio State Univ., Columbus, OH, 43210, USA
SOURCE: Prostaglandins, Leukotrienes and Medicine (1986), 23(2-3), 129-34
CODEN: PLMEDD; ISSN: 0262-1746
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Human platelets metabolize 7,10,13,16-docosatetraenoic acid [28874-58-0] and 4,7,10,13,16-docosapentaenoic acid [25182-74-5] into C22

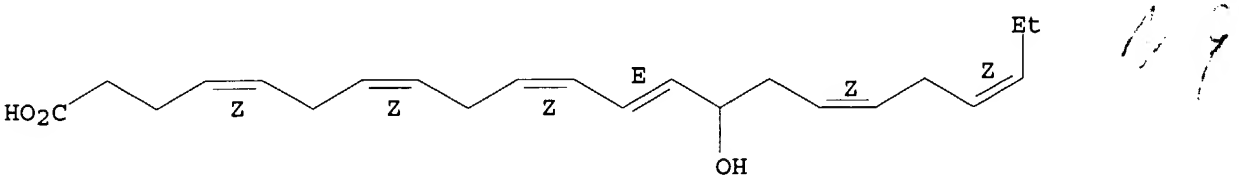
thromboxanes, C19 hydroxyheptadecatrienoic acid analogs, and 14-hydroxy fatty acids via the lipoxygenase [9029-60-1] pathway. Conversely, the 2 analogous (n-3) acids, 7,10,13,16,19-docosapentaenoic acid [24880-45-3] and 4,7,10,13,16,19-docosahexaenoic acid [6217-54-5] are metabolized only into a pair of isomeric 11- and 14-hydroxy fatty acids. Apparently, platelets contain >1 lipoxygenase.

IT **87042-40-8**
RL: FORM (Formation, nonpreparative)
(formation of, by blood platelets of humans, thromboxanes in relation to)

RN 87042-40-8 HCAPLUS

CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L28 ANSWER 51 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1986:104814 HCAPLUS

DOCUMENT NUMBER: 104:104814

TITLE: Lipoxygenase in trout gill tissue acting on arachidonic, eicosapentaenoic and docosahexaenoic acids

AUTHOR(S): German, J. Bruce; Bruckner, Geza G.; Kinsella, John E.

CORPORATE SOURCE: Inst. Food Sci., Cornell Univ., Ithaca, NY, 14853, USA

SOURCE: Biochimica et Biophysica Acta (1986), 875(1), 12-20
CODEN: BBACAQ; ISSN: 0006-3002

DOCUMENT TYPE: Journal

LANGUAGE: English

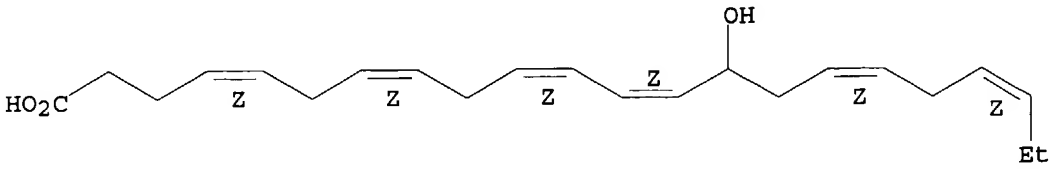
AB Lipoxygenase activity was characterized in the gill tissue of freshwater trout. Incubation of arachidonic acid with gill prepns. yielded 12-hydroxyeicosatetraenoic acid as the major product, suggesting a 12-lipoxygenase. Eicosapentaenoic acid was similarly converted to 12-hydroxyeicosapentaenoic acid. Both arachidonic acid and docosahexaenoic acid were converted with equal apparent velocities and affinities into single monohydroxy derivs. Analyses of the hydroxy product of docosahexaenoic acid were consistent with 14-hydroxydocosahexaenoic acid. This enzyme activity was localized to the cytosolic fraction and displayed a broad pH optimum around pH 7. The enzyme was insensitive to the cyclooxygenase inhibitors indomethacin and aspirin, but activity was strongly inhibited in the presence of the lipoxygenase inhibitors SnCl2 (5 mM), esculetin (10 μM), and eicosatetraynoic acid (100 μM).

IT **100838-25-3**
RL: FORM (Formation, nonpreparative)
(formation of, by lipoxygenase of gill of lake trout)

RN 100838-25-3 HCAPLUS

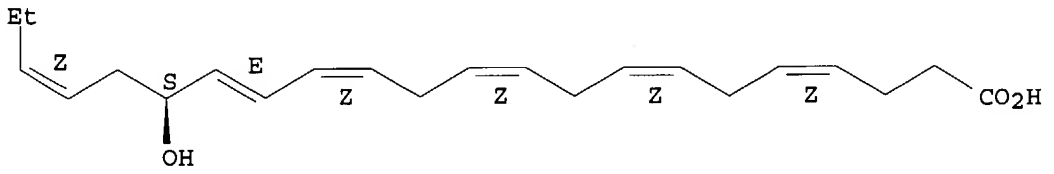
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (all-Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L28 ANSWER 52 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1984:586797 HCAPLUS
DOCUMENT NUMBER: 101:186797
TITLE: Inhibition of platelet 12-lipoxygenase by hydroxy-fatty acids
AUTHOR(S): Mitchell, Paul D.; Hallam, Catherine; Hemsley, Paul E.; Lord, Garry H.; Wilkinson, David
CORPORATE SOURCE: Dep. Biochem., Fisons PLC, Loughborough/Leics., LE11 0RH, UK
SOURCE: Biochemical Society Transactions (1984), 12(5), 839-41
CODEN: BCSTB5; ISSN: 0300-5127
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Nine C(n-6)-hydroxy fatty acids were biosynthesized from unsatd. fatty acid precursors and tested as inhibitors of human blood platelet arachidonate 12-lipoxygenase (I). Five of the unsatd. hydroxy fatty acids were inactive as inhibitors and the other 4 gave IC50 values of <10 μM. None of the compds. inhibited prostaglandin synthetase and none were metabolized by I. The suggestion that some hydroxy fatty acids may have a regulatory function in the I pathway of arachidonate metabolism is supposed by these results.
IT **92693-03-3**
RL: BIOL (Biological study)
(arachidonate 12-lipoxygenase of human blood platelets inhibition by)
RN 92693-03-3 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, [S-(E,Z,Z,Z,Z,Z)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L28 ANSWER 53 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1984:436621 HCAPLUS
DOCUMENT NUMBER: 101:36621
TITLE: Uptake, release and metabolism of docosahexaenoic acid (DHA, C22:6ω3) in human platelets and neutrophils
AUTHOR(S): Fischer, S.; Von Schacky, C.; Siess, W.; Strasser, T.; Weber, P. C.
CORPORATE SOURCE: Med. Klin. Innenstadt, Univ. Muenchen, Munich, 8000/2, Fed. Rep. Ger.
SOURCE: Biochemical and Biophysical Research Communications

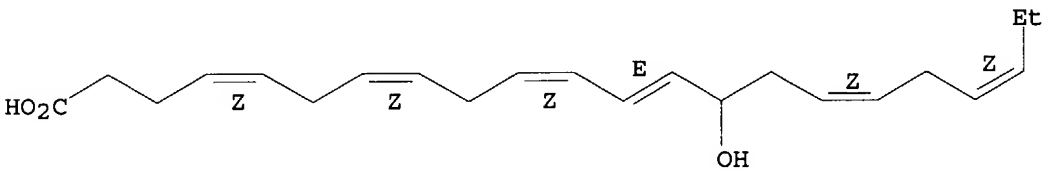
(1984), 120(3), 907-18
CODEN: BBRCA9; ISSN: 0006-291X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Exogenous DHA is converted by human platelets to 14- and 11-hydroxydocosahexaenoic acid (HDHE) and by human neutrophils mainly to 7-HDHE. Human platelets prelabeled with [1414C]DHA,14 [14C]-eicosapentaenoic acid (EPA) and [14C14]-arachidonic acid (AA) and stimulated with thrombin released and metabolized DHA only in trace amts. as compared to EPA and AA. [1414C]DHA is incorporated into the 2-position of platelet phospholipids and occurs predominantly in phosphatidylethanolamine. DHA and EPA were also incorporated by dietary means into phospholipids of platelets and neutrophils. In resting platelets free DHA as well as free AA and EPA are not detectable. In platelets stimulated ex vivo with thrombin DHA is not significantly released which is in contrast to EPA and AA. After stimulation, 14-HDHE is found only in trace amts. as compared to 12-hydroxyeicosapentaenoic and 12-hydroxyeicosatetraenoic acid. In DHA enriched neutrophils formation of HDHEs cannot be demonstrated after stimulation with ionophore A 23187. Thus, even after dietary enrichment of DHA in phospholipids of platelets and neutrophils the level of free DHA and/or formation of HDHEs might be too low to substantially affect arachidonic acid metabolism and related functions of these cells.

IT **87042-40-8**
RL: FORM (Formation, nonpreparative)
(formation of, from docosahexaenoic acid by blood platelet and neutrophils of human)

RN 87042-40-8 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



L28 ANSWER 54 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1984:435331 HCAPLUS
DOCUMENT NUMBER: 101:35331
TITLE: Autooxidation of docosahexaenoic acid: analysis of ten isomers of hydroxydocosahexaenoate
AUTHOR(S): VanRollins, Mike; Murphy, Robert C.
CORPORATE SOURCE: Health Sci. Cent., Univ. Colorado, Denver, CO, 80262, USA
SOURCE: Journal of Lipid Research (1984), 25(5), 507-17
CODEN: JLPRAW; ISSN: 0022-2275
DOCUMENT TYPE: Journal
LANGUAGE: English

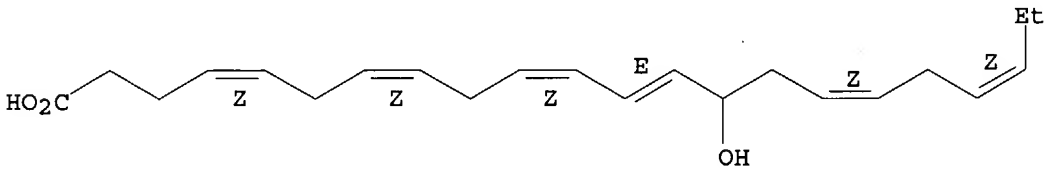
AB Docosahexaenoic acid, an n-3 essential fatty acid, is enzymically converted by platelets, basophils, and liver microsomes into metabolites containing conjugated diens with allylic hydroxyl groups. To help identify these metabolites, stds. were prepared by autoxidn. of docosahexaenoic acid. After isolation by reverse phase and normal phase high-performance chromatog. (HPLC), 10 hydroxy isomers of docosahexaenoic acid were

identified by capillary gas-liquid chromatog., UV spectroscopy, and mass spectrometry. From these studies and reported elution orders for similar metabolites derived from linoleic, linolenic, and arachidonic acids, 2 basic HPLC elution patterns became apparent. Under reverse phase chromatog. conditions, the distance of the trans-double bond from the carboxyl group was the critical parameter in determining the elution order. Under silicic acid chromatog. conditions, the distance of the hydroxyl from the carbomethoxy group seemed to determine the elution order. The dramatic difference in selectivity between reverse and normal phase HPLC of the hydroxy acids provides critical information useful for identifying endogenous metabolites.

IT **87042-40-8P 90780-51-1P 90780-52-2P**
90780-53-3P 90906-41-5P
RL: PREP (Preparation)
(preparation and characterization of, as docosahexaenoic acid autoxidn. product)

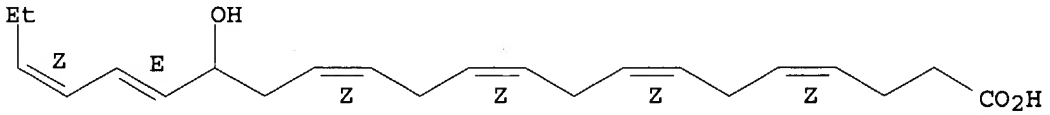
RN 87042-40-8 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



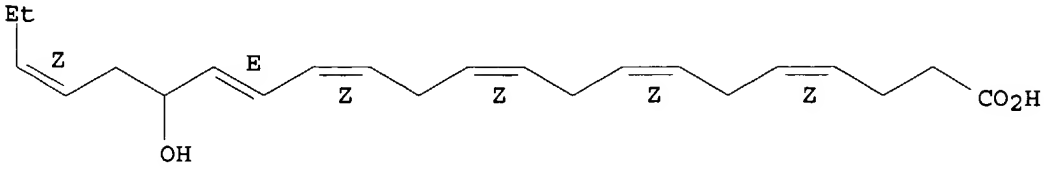
RN 90780-51-1 HCAPLUS
CN 4,7,10,13,17,19-Docosahexaenoic acid, 16-hydroxy-, (4Z,7Z,10Z,13Z,17E,19Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



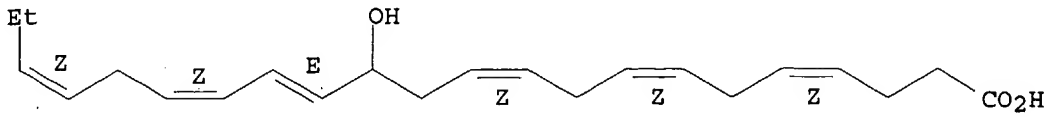
RN 90780-52-2 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, (4Z,7Z,10Z,13Z,15E,19Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 90780-53-3 HCAPLUS
CN 4,7,10,14,16,19-Docosahexaenoic acid, 13-hydroxy-, (4Z,7Z,10Z,14E,16Z,19Z)- (9CI) (CA INDEX NAME)

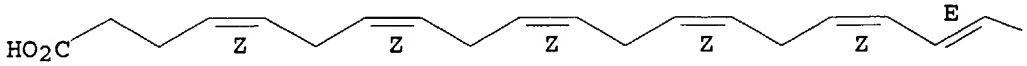
Double bond geometry as shown.



RN 90906-41-5 HCAPLUS
CN 4,7,10,13,16,18-Docosahexaenoic acid, 20-hydroxy-, (4Z,7Z,10Z,13Z,16Z,18E)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



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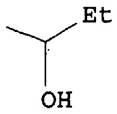
PAGE 1-B



L28 ANSWER 55 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1984:419194 HCAPLUS
DOCUMENT NUMBER: 101:19194
TITLE: Oxidation of docosahexaenoic acid by rat liver microsomes
AUTHOR(S): VanRollins, Mike; Baker, Rodney C.; Sprecher, Howard W.; Murphy, Robert C.
CORPORATE SOURCE: Health Sci. Cent., Univ. Colorado, Denver, CO, 80262, USA
SOURCE: Journal of Biological Chemistry (1984), 259(9), 5776-83
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: English

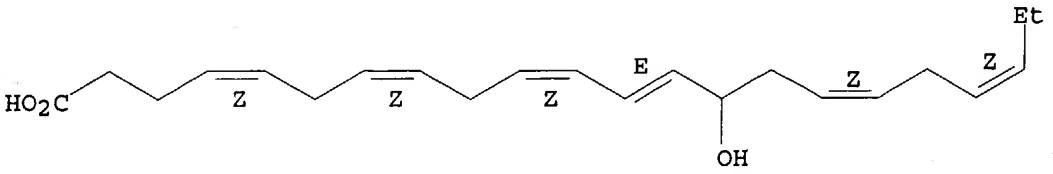
AB [1-14C]docosahexaenoic acid (n-3) was incubated at 37° for 30 min in the presence of rat liver microsomes and 1 mM NADPH. The products were isolated by using organic solvent extns., and reverse phase and normal phase HPLC. Isolates were identified by UV spectroscopy, capillary gas-liquid chromatog., and gas chromatog.-mass spectrometer. The major metabolites were: 19,20-, 16,17-, 13,14-, 10,11-, and 7,8-dihydroxydocosapentaenoic acids, 22-hydroxydocosahexaenoic acid, and 21-hydroxydocosahexaenoic acid. The minor metabolites were 17-hydroxy-4,7,10,13,15,19-, 16-hydroxy-4,7,10,17,19-, 14-hydroxy-4,7,10,12,-16,19-, 13-hydroxy-4,7,10,14,16,19-, 11-hydroxy-4,7,9,13,16,19-, 10-hydroxy-4,7,11,13,16,19-,8-hydroxy-4,6,10,13,16,19-, and 7-hydroxy-4,8,10,13,16,19-docosahexaenoic acids. These metabolites of docosahexaenoic acid resulted from 4 distinct classes of oxidation, ω-hydroxylations, (ω-1)-hydroxylations, epoxidns., and lipoxygenase-like hydroxylations. The similarity of these product

profiles to those reported for comparable microsomal incubations with other essential fatty acids suggest that microsome cytochrome P 450 monooxygenases were involved.

IT **87042-40-8 90780-51-1 90780-52-2 90780-53-3**
RL: BIOL (Biological study)
(as product of docosahexaenoate oxidation by liver microsomes)

RN 87042-40-8 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)-(9CI) (CA INDEX NAME)

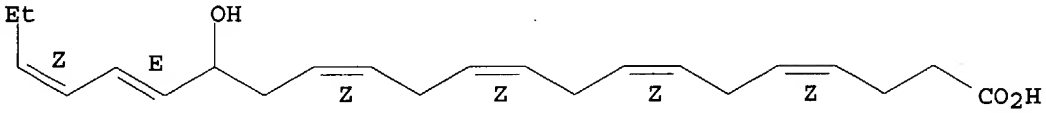
Double bond geometry as shown.



29

RN 90780-51-1 HCAPLUS
CN 4,7,10,13,17,19-Docosahexaenoic acid, 16-hydroxy-, (4Z,7Z,10Z,13Z,17E,19Z)-(9CI) (CA INDEX NAME)

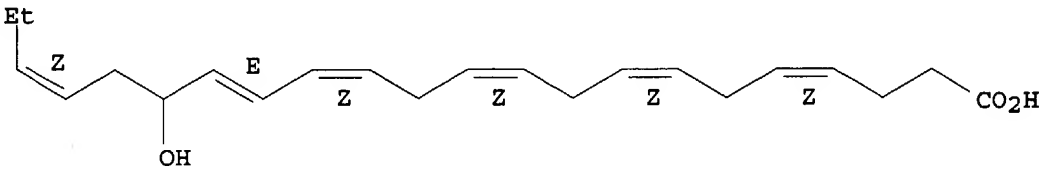
Double bond geometry as shown.



33

RN 90780-52-2 HCAPLUS
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, (4Z,7Z,10Z,13Z,15E,19Z)-(9CI) (CA INDEX NAME)

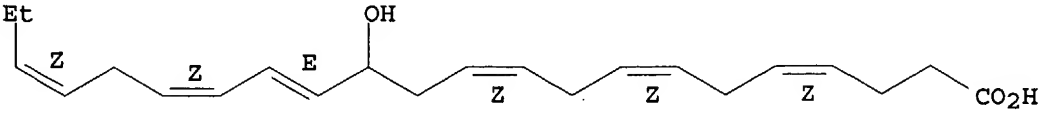
Double bond geometry as shown.



30

RN 90780-53-3 HCAPLUS
CN 4,7,10,14,16,19-Docosahexaenoic acid, 13-hydroxy-, (4Z,7Z,10Z,14E,16Z,19Z)-(9CI) (CA INDEX NAME)

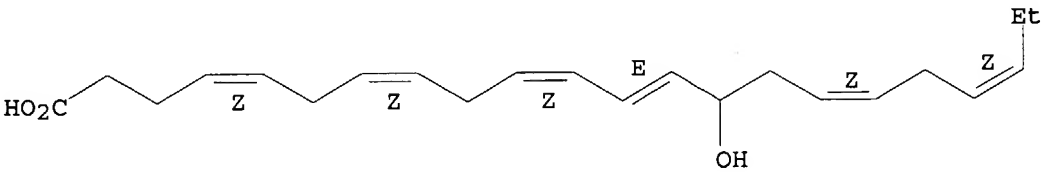
Double bond geometry as shown.



28

L28 ANSWER 56 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1983:519889 HCAPLUS
DOCUMENT NUMBER: 99:119889
TITLE: Synthesis of hydroxy fatty acids from 4,7,10,13,16,19-[1-14C]docosahexaenoic acid by human platelets
AUTHOR(S): Aveldano, Marta I.; Sprecher, Howard
CORPORATE SOURCE: Coll. Med., Ohio State Univ., Columbus, OH, 43210, USA
SOURCE: Journal of Biological Chemistry (1983), 258(15), 9339-43
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Human platelets incubated in the presence of 54 μM [1-14C]22:6 produced hydroxydocosahexaenoic acid (HDHE) at .apprx.1/2 the rate with which 12-hydroxy-5,8,10,14-eicosatetraenoic acid is produced from [1-14C]arachidonic acid. More than 90% of the radioactivity in HDHE was distributed among 2 major isomers, 14-HDHE and 11-HDHE. The production of HDHEs was unaffected by indomethacin but completely inhibited by 5,8,11,14-heneicosatetraynoic acid, which suggests that the hydroxy fatty acids are produced by lipoxygenase. The proportions of HDHE isomers varied with the concentration of 22:6. The ratio 14-HDHE/11-HDHE was higher at 6.8 μM 22:6 than when platelets were incubated with 54 μM 22:6. Thus, the amts. of these isomers produced depend both on the availability of 22:6 as well as on competition of this acid with other acids for lipoxygenase.
IT **87042-40-8**
RL: FORM (Formation, nonpreparative)
(formation of, from docosahexaenoate by human blood platelets)
RN 87042-40-8 HCAPLUS
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



29

L28 ANSWER 57 OF 57 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1979:434198 HCAPLUS
DOCUMENT NUMBER: 91:34198
TITLE: Substrate specificity for the synthesis of cyclic fatty acids by a flaxseed extract
AUTHOR(S): Vick, Brady A.; Zimmerman, Don C.
CORPORATE SOURCE: Dep. Biochem., North Dakota State Univ., Fargo, ND, 58105, USA
SOURCE: Plant Physiology (1979), 63(3), 490-4
CODEN: PLPHAY; ISSN: 0032-0889
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 12-Oxo-cis-10,15-phytodienoic acid (I) is an enzymic product obtained from incubations of (9,12,15)-linolenic acid with exts. of flaxseed (Linum usitatissimum). 13-L-Hydroperoxy-cis-9,15-trans-11-octadecatrienoic acid, a product of lipoxygenase catalysis, was an intermediate in the enzymic

synthesis of I. Substrate specificity studies showed that n-3,6,9 unsatn. is an absolute requirement for conversion of polyunsatd. fatty acids into analogous products containing a cyclopentenone ring. Fatty acids with 18, 20, or 22 carbons that satisfied this requirement were effective substrates. The optimum activity of the enzyme from flaxseed was at pH 7.2.

IT **70596-95-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, by flaxseed enzymic extract)

RN 70596-95-1 HCAPLUS

CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroperoxy-, (4Z,7Z,10Z,13Z,15E,19Z)- (9CI) (CA INDEX NAME)

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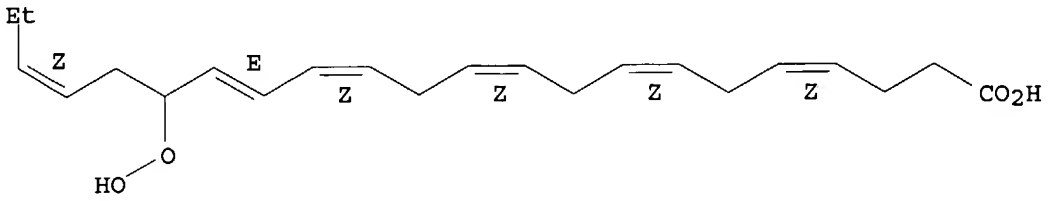

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L17                STR
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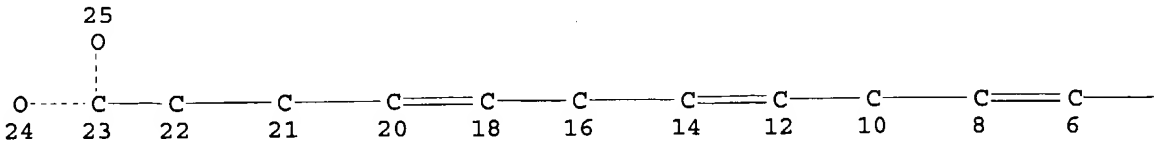
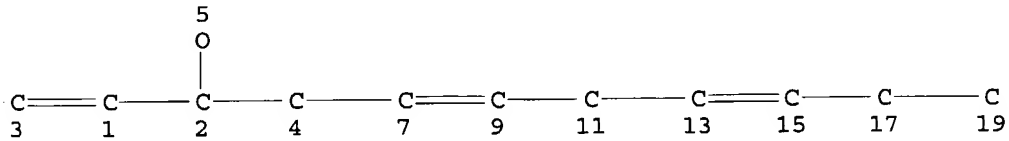


Page 1-A



Page 1-B
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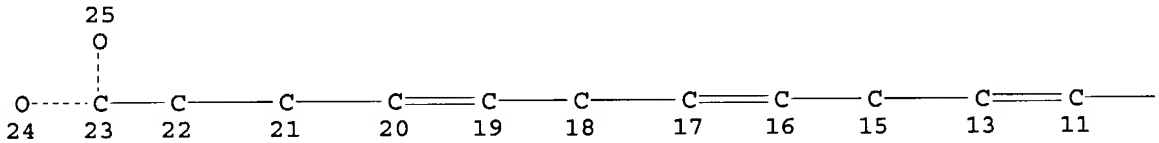
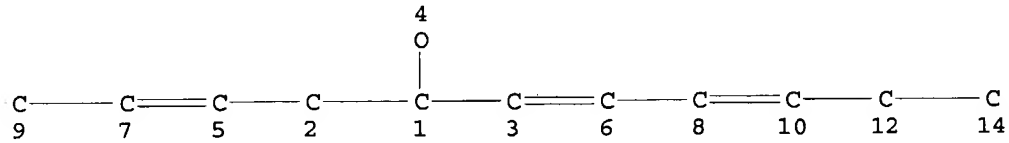
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE
L20 STR



Page 1-A



Page 1-B
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NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE
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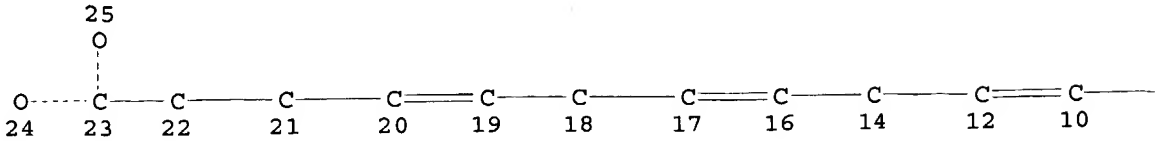
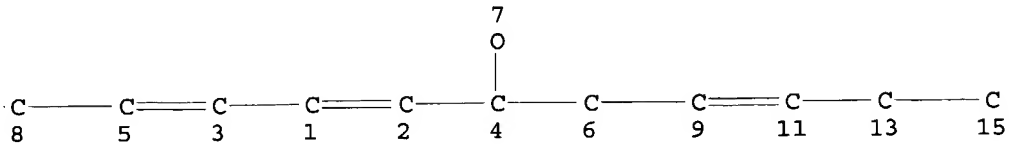


Page 1-A



Page 1-B
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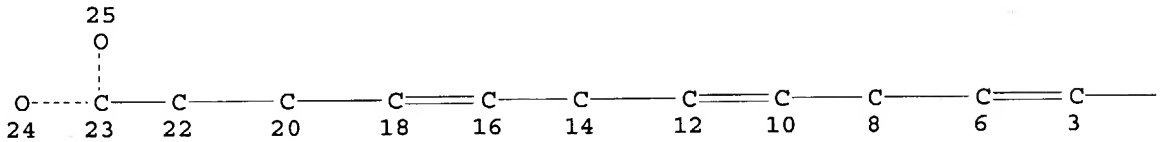
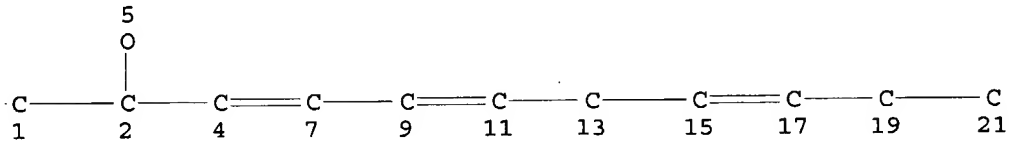


Page 1-A



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NODE ATTRIBUTES:
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NUMBER OF NODES IS 25

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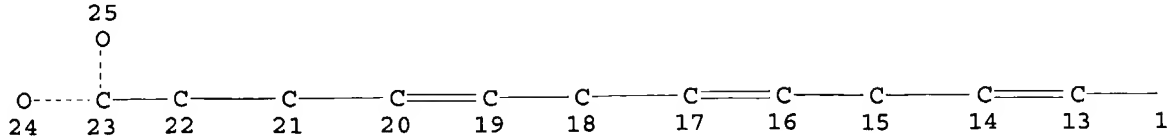

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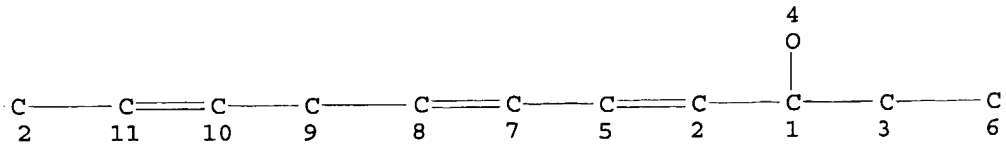

Page 1-B
NODE ATTRIBUTES:
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DEFAULT ECLEVEL IS LIMITED

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NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE
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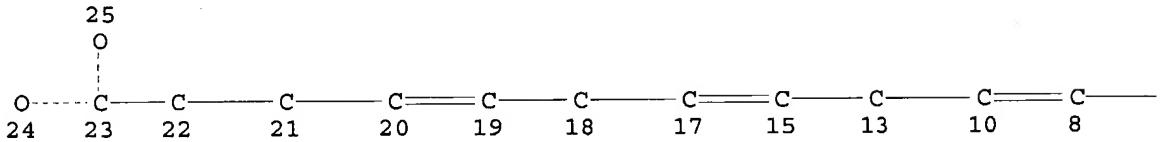
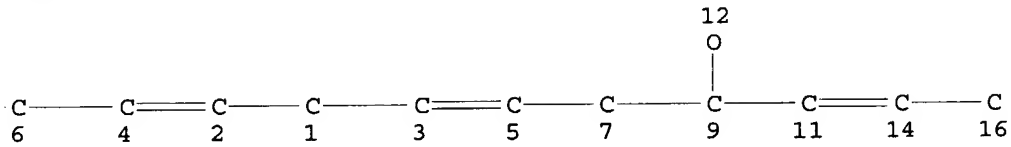


Page 1-A



Page 1-B
NODE ATTRIBUTES:
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DEFAULT ECLEVEL IS LIMITED

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NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE
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